

# $d$ -Wave Pairing Driven by Bipolaric Modes Related to Giant Electron-Phonon Anomalies in High- $T_c$ Superconductors

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## Abstract

Taking into account microscopic properties of most usual high- $T_c$  superconductors, like cuprates, we define a class of microscopic model Hamiltonians for two fermions (electrons or holes) and one boson (bipolaron) on the two-dimensional square lattice. We establish that these model Hamiltonians can show  $d$ -wave pairing at the bottom of their spectrum, despite their space isotropy. This phenomenon appears when a “giant electron-phonon anomaly” is present at the boundaries of the Brillouin zone (“half breathing” bond-stretching mode), like in doped cuprates. Our results can be used to derive effective electron-electron interactions mediated by bipolarons and we discuss regimes where the corresponding model is relevant for the physics of high-temperature superconductivity and can be mathematically rigorously studied.

Keywords: High  $T_c$ , Superconductivity, Hubbard model, BCS model,  $d$ -wave,  $s$ -wave, Bipolaron

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# 1 Introduction

Cuprates and many other superconducting materials with high critical temperatures have features which are non–usual as compared to conventional superconductors. Quoting [1]:

*High–temperature superconductivity in the copper oxides, first discovered twenty years ago, has led researchers on a wide-ranging quest to understand and use this new state of matter. From the start, these materials have been viewed as “exotic” superconductors, for which the term exotic can take on many meanings. The breadth of work that has taken place reflects the fact that they have turned out to be exotic in almost every way imaginable. They exhibit new states of matter ( $d$ –wave superconductivity, charge stripes), dramatic manifestations of fluctuating superconductivity, plus a key inspiration and testing ground for new experimental and theoretical techniques.*

Some of these “exotic” properties, as for instance the  $d$ -wave pairing and density waves (charge stripes) mentioned above, turn out to be common to many high- $T_c$  superconductors, in particular to those based on cuprates [1]. Hence, the understanding of generic microscopic structures leading to that typical behavior can reveal mechanisms behind high-temperature superconductivity.

In fact, the microscopic foundations of high- $T_c$  superconductivity are still nowadays a subject of much debate. In the present paper we would like to address this issue by analyzing a specific three-body problem. Indeed, we have following aims:

- Taking into account microscopic properties of most usual high- $T_c$  superconductors (in particular cuprates), as found in recent experiments, we define a class of *microscopic* model Hamiltonians for two fermions (electrons or holes) and one boson (bipolaron) on the two-dimensional square lattice.
- We mathematically rigorously analyze the spectral projection on the bottom of the spectrum of model Hamiltonians and identify the range of parameters that leads to  $d$ -wave pairing.
- We use the properties of such spectral projections in order to derive an effective model, here called “effective uncoupled model”, in which the two species, bosons and fermions, do not interact with each other.

Our main mathematical assertions are Theorems 2, 3, 4 and Corollary 5. The paper is organized as follows:

- Based on experimental facts about typical high- $T_c$  superconductors (like cuprates), Section 2 gives and discusses assumptions on model Hamiltonians.
- Section 3 formulates the mathematical setting and our main results. In particular, we establish that model Hamiltonians *which are invariant with respect to  $90^\circ$ -rotations* can show  $d$ -wave pairing at the bottom of their spectrum.
- We derive the effective uncoupled many-body model in Section 4, using results of Section 3. This is reminiscent of the derivation of the BCS model where the attraction between electrons is mediated by bosonic degrees of freedom (e.g. phonons). See also the Fröhlich model. The way we do it is however different from the usual derivations and is mathematically rigorous

in the 2-fermions–1-boson sector. Moreover, this new model can explain  $d$ -wave superconductivity, in contrast to the BCS model<sup>1</sup>.

- Section 5 gathers technical proofs on which Sections 3–4 are based.
- Section 6 is an appendix on direct integral decompositions and the Birman–Schwinger principle, which are important technical tools to prove our assertions.

### Notation 1

*To simplify notation, we denote positive and finite constants by  $D \in (0, \infty)$ . These constants do not need to be the same from one statement to another. We denote the Banach space of bounded operators acting on a Hilbert space  $\mathcal{H}$  by  $\mathcal{B}(\mathcal{H})$  with operator norm  $\|\cdot\|_{\text{op}}$  and identity  $1_{\mathcal{H}}$ .*

## 2 Prototypical Properties of High- $T_c$ Superconductors

In the next four subsections we briefly discuss some experimental facts giving, in our opinion, important hints about the nature of the microscopic interaction involving electrons in superconducting cuprates. Based on this discussion, we propose a list of assumptions on our model Hamiltonians.

### 2.1 Electron Repulsion and Hoppings

It is well-known that undoped cuprates are insulators. Moreover, experiments showed that the insulating phase of cuprates is indeed a so-called “Mott insulating phase”. See for instance [1] for a review. This phase is characterized by a periodic distribution of electrons with exactly one particle per lattice site. Such a space distribution of electrons is a consequence of a strong repulsion of two charge particles sitting at the same lattice site. Dopping cuprates with holes or electrons leads to a mean density  $\rho$  different from one electron per site and the above configuration is not anymore energetically favorable. It turns out that, in this case, at sufficiently small temperatures, the superconducting phase is the one minimizing

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<sup>1</sup>Note that many authors contributed to the mathematics of the (usual) BCS-model. For instance, to mention some of them: Haag, Thirring, Lieb, Bogoliubov (Jr), Zagrebnov, or more recently Seiringer and Hainzl, etc.

the free-energy density. In particular, the system undergoes a phase transition and becomes a superconductor. This phenomenon was rigorously proven in [2] for the strong coupling reduced BCS Hamiltonian perturbed by a repulsive Hubbard interaction. Further properties of the phase diagram of real cuprates are also captured if we consider the two-band version of this Hamiltonian. In fact, for real cuprates the phase diagram is not symmetric with respect to the axis  $\rho = 1$  (no doping, one electron per site). The critical temperature tends to be higher for hole doping than for electron doping. This property is shown to be true for the two-band model studied in [3].

The results of [2, 3] confirm, from a mathematical point of view, that the shape of the typical phase diagram of cuprates as well as the corresponding type of phase transition can be drawn back to the competition between a strongly repulsive short-range force between electrons and a weak but long-range BCS-type interaction. We thus assume the following:

**Assumption 1 (Hubbard repulsion)**

*The repulsive force between two near-lying electrons is represented by the usual Hubbard repulsive interaction (which does not vanish only for particles at the same lattice site).*

The absence of hopping terms in the Hamiltonian studied in [2, 3] corresponds to the so-called “strong coupling approximation” for the BCS model. Here, we aim to introduce general hopping terms in our models. Note however that the “strong coupling regime” is, from one side, technically convenient, but, first of all, also the most relevant case in which concerns high- $T_c$  superconductivity: Experiments suggest [4] that the inter-particle interaction energy is five to eight times bigger than the hopping strength:

**Assumption 2 (Strong coupling regime)**

*The interactions between particles are strong with respect to the hopping amplitudes.*

Charge transport in cuprates take place within separated (almost) independent layers. In fact, we focus on high- $T_c$  materials for which superconducting carriers, mainly holes in the case of cuprates, move within two-dimensional  $\text{CuO}_2$  layers made of  $\text{Cu}^{++}$  and  $\text{O}^{--}$ , see, e.g., [4, Fig. 5.3. p. 127]. The following assumption is thus reasonable:

**Assumption 3 (Two-dimensionality)**

*The charge transport occurs within independent two-dimensional layers.*

We also know from [2, 3] that the reduced BCS interaction, also in presence of the Hubbard repulsive term, always lead to  $s$ -wave pairing of electrons in the superconducting phase. Hence, this component should be replaced by another effective long-range attractive force. Effective microscopic forces between electrons, which could play a role in the phenomenon of  $d$ -wave pairing, are deduced in Section 4 from results of Section 3. One important physical fact that gives hint on the nature of the microscopic forces leading to high-temperature superconductivity are the anomalous dispersion relations of phonons in high- $T_c$  superconductors discussed in the following subsection.

## 2.2 Giant Electron-Phonon Anomalies in Doped Cuprates

Anomalous dispersion relations of phonons, i.e., dispersion relations of a form not expected from lattice-dynamical models, are usually due to the coupling of phonon to electrons. Such a phenomenon is observed even in conventional metals. In doped cuprates and other high- $T_c$  superconductors such an anomaly is very strong (“giant electron-phonon anomaly”) and very localized in specific regions of the Brillouin zone, suggesting a strong interaction between elastic and charged modes in some small range of quasi-momenta. For a recent review on giant electron-phonon anomalies in doped cuprates see for instance [5]. Experiments with cuprates show that these anomalies get stronger at the boundaries of the Brillouin zone (“half breathing” bond-stretching mode) as the doping is increased [6]. Since, until a certain point, the increasing of doping also increases the superconducting critical temperature, it is natural to expect that a strong coupling between charged and “half breathing” bond-stretching modes is part of the mechanism leading to high temperature superconductivity [7]. In a two-dimensional model for superconductors “half breathing” bond-stretching modes correspond to  $(\pm\pi, 0)$  and  $(0, \pm\pi)$  quasi-momentum transfers.

The precise type of coupling between charged and elastic modes responsible for the giant electron-phonon anomalies is a subject of debate. One possible mechanism is the existence incipient instability due to the formation of polarons and bipolarons [8, 9, 10, 11, 12]. For other mechanisms see the review [5]. In the next subsection we discuss the bipolaronic scenario in more details. The following physical assumption, that is, strong bipolaron instabilities at quasi-momenta  $(\pm\pi, 0)$  and  $(0, \pm\pi)$ , is made with respect to the two-dimensional microscopic models we consider:

**Assumption 4 (Strong bipolaron instabilities)**

*The strong interaction between elastic and charged modes at half breathing bond-stretching modes is related to the formation of bipolarons.*

We also assume the following condition:

**Assumption 5 (Zero-spin bipolarons)**

*The total spin of bipolarons is zero.*

Considering spin-one bipolarons would also be feasible, but we refrain from doing it for simplicity.

**2.3 Bipolaron–Electron Exchange Interaction**

There are experimental evidences of polaron and bipolaron formation in high- $T_c$  superconductors, even in insulating and metallic phases. See, for instance, [13] for a brief review on these experimental issues. Some efforts have been made to theoretically explain high- $T_c$  superconductivity by assuming that bipolarons, and not Cooper pairs, are the main charge carriers in the superconducting phase [14, 15]. Recall that it is experimentally known that, for cuprates and other high- $T_c$  superconductors, the charge carriers in the superconducting phase have two times the charge of the electron, as in the case of conventional superconductors. Nevertheless, there is an important objection to this picture: polarons and bipolarons (more generally,  $n$ -polarons,  $n \in \mathbb{N}$ ) are charge carriers that are self-trapped inside a strong and local lattice deformation that surrounds them (their are electrons “dressed with phonons”). Such strong lattice deformations attached to bipolarons can hardly move and this is not in accordance with the known mobility of superconducting charge carriers. Hence we assume:

**Assumption 6 (Small bipolaron mobility)**

*The hopping strength of bipolarons (bosonic particles) is very small or even negligible.*

One way out of this mobility problem is to assume that bipolarons can decay into two-electrons and, reciprocally, two moving electrons can bind together to form a new bipolaron [13]:

**Assumption 7 (Bipolaron–electron exchange)**

*Bipolarons can decay into two electrons and moving electrons can bind to form*

*bipolarons. This exchange process is strong for quasi-momenta near the half breathing bond-stretching modes, i.e., in two-dimensions,  $(\pm\pi, 0)$ ,  $(0, \pm\pi)$ , and weak away from these singular points.*

This exchange process allows a good mobility of charge carriers because the electronic state has a non-negligible hopping strength. Moreover, such a boson-fermion exchange process effectively creates an attractive force between electrons, like in the Fröhlich model for conventional superconductivity. So, we expect a binding mechanism for electron pairs similar, in a sense, to the Cooper pairing, but with the mediating boson being a bipolaron instead of (directly) a phonon.

As the exchange process described above is concentrated (in momentum space) around a few isolated points (half breathing bond-stretching modes) of the Brillouin zone, it is conceivable that the following holds true:

**Assumption 8 (Long-range effective forces)**

*The forces between electrons mediated by bipolarons are long-ranged (in space).*

This assumption is not in contradiction with the experimentally known fact that the pairs responsible for charge transport in high- $T_c$  superconductors have (in contrast to conventional superconductors) a very small extension. Indeed, as shown in [2], the small space extension of superconducting pairs is rather due to the strong coupling regime. Note moreover that Assumption 8 is not used in Section 3. It is only relevant for the effective many-body model we propose in Section 4.

## 2.4 Space Isotropy

There are theoretical studies showing that an anisotropic phonon-electron (or, more generally, boson-fermion) interaction can explain  $d$ -wave pairing of electrons [16]. On the other hand, there is absolutely no evidence of such an anisotropy in cuprates, see [5] for instance. So, we aim to derive  $d$ -pairing (among other phenomena typical to high- $T_c$  superconductors) from strictly isotropic models and we assume the following:

**Assumption 9 (Isotropy of interactions)**

*The interactions are invariant under lattice translations, reflections and  $90^\circ$ -rotations.*

This condition concludes the list of assumptions on which we base our mathematically rigorous study.



### 3 Mathematical Setting and Main Results

In this section, we mathematically implement (the physical) Assumptions 1–7 and 9.

#### 3.1 Bipolaron–Electron Model for High– $T_c$ Superconductors

By taking into account all model assumptions formulated above, we propose below a Hamiltonian for bosons and fermions in the  $\mathbb{Z}^2$ –lattice. In particular, the host material supporting particles is assumed to be a (perfect) two–dimensional cubic crystal (cf. Assumption 3).

For any  $n \in \mathbb{N}$ , let  $\mathcal{S}_{n,\pm}$  be the orthogonal projections onto the subspace of, respectively, antisymmetric (–) and symmetric (+)  $n$ –particle wave functions in  $\mathfrak{h}_{\pm}^{\otimes n}$ , the  $n$ –fold tensor product of either  $\mathfrak{h}_{-} := \ell^2(\mathbb{Z}^2; \mathbb{C}^2)$  or  $\mathfrak{h}_{+} := \ell^2(\mathbb{Z}^2; \mathbb{C})$ . Let  $\mathfrak{h}_{n,\pm} := \mathcal{S}_{n,\pm} \mathfrak{h}_{\pm}^{\otimes n}$  for all  $n \in \mathbb{N}$ ,  $\mathfrak{h}_{0,\pm} := \mathbb{C}$ , and define

$$\mathcal{F}_{\pm} := \bigoplus_{n=0}^{\infty} \mathfrak{h}_{n,\pm}$$

to be respectively the fermion ((–), spin 1/2) and boson ((+), spinless, cf. Assumptions 4 and 5) Fock spaces. The Hilbert space of the compound system is thus

$$\mathcal{F}_{-,+} := \mathcal{F}_{-} \otimes \mathcal{F}_{+} \simeq \bigoplus_{n,m=0}^{\infty} \mathfrak{h}_{m,-} \otimes \mathfrak{h}_{n,+} .$$

Here,  $\simeq$  denotes the existence of a *canonical* isomorphism of Hilbert spaces. A dense subset of  $\mathcal{F}_{-,+}$  is given by the subspace

$$\mathcal{D} := \text{span} \left\{ \bigcup_{m,n \in \mathbb{N}_0} \mathfrak{h}_{m,-} \otimes \mathfrak{h}_{n,+} \right\} . \quad (1)$$

The creation and annihilation operators are denoted by

$$a_{x,s}^* \equiv a_{x,s}^* \otimes \mathbf{1}_{\mathcal{F}_{+}} , \quad a_{x,s} \equiv a_{x,s} \otimes \mathbf{1}_{\mathcal{F}_{+}} , \quad x \in \mathbb{Z}^2, \quad s \in \{\uparrow, \downarrow\} ,$$

for fermions and

$$b_x^* \equiv \mathbf{1}_{\mathcal{F}_{-}} \otimes b_x^* , \quad b_x \equiv \mathbf{1}_{\mathcal{F}_{-}} \otimes b_x , \quad x \in \mathbb{Z}^2 ,$$

in the boson case.

The fermionic part of the (infinite volume) Hamiltonian is defined on the dense subspace  $\mathcal{D} \subset \mathcal{F}_{-,+}$  by the symmetric operator

$$H_f := \epsilon \left( -\frac{1}{2} \sum_{s \in \{\uparrow, \downarrow\}, x, y \in \mathbb{Z}^2, |x-y|=1} a_{x,s}^* a_{y,s} + 2 \sum_{s \in \{\uparrow, \downarrow\}, x \in \mathbb{Z}^2} a_{x,s}^* a_{x,s} \right) + U \sum_{x \in \mathbb{Z}^2} n_{x,\uparrow} n_{x,\downarrow} \quad (2)$$

with  $\epsilon, U \geq 0$ . The first term of this operator represents, as usual, next-neighbor hoppings of fermions on the  $\mathbb{Z}^2$ -lattice. More generally, we could take a term of the form

$$\epsilon \sum_{s \in \{\uparrow, \downarrow\}, x, y \in \mathbb{Z}^2} h_f(|x-y|) a_{x,s}^* a_{y,s} ,$$

for some real-valued function  $h_f$  satisfying

$$\sum_{x \in \mathbb{Z}^2} |h_f(x)| < \infty .$$

We refrain from considering this general case for simplicity, only, but our study can be easily generalized to this situation. The last term of (2) stands for the (screened) Coulomb repulsion as in the celebrated Hubbard model. So, the parameter  $U$  is a positive number, i.e.,  $U \geq 0$ . See Assumption 1. The parameter  $\epsilon \geq 0$  represents the relative strength of the hopping amplitude with respect to the interparticle interaction. In high- $T_c$  superconductors,  $\epsilon$  is expected to be relatively small. Cf. Assumption 2.

The bosonic part of the Hamiltonian is meanwhile defined on  $\mathcal{D}$  by

$$H_b := \epsilon \left( -\frac{h_b}{2} \sum_{x, y \in \mathbb{Z}^2, |x-y|=1} b_x^* b_y + 2h_b \sum_{x \in \mathbb{Z}^2} b_x^* b_x \right) , \quad (3)$$

where  $h_b \geq 0$  is very small or even zero (cf. Assumption 6). This symmetric operator does not include any density-density interaction. Indeed, we only consider below the one-boson subspace and such interactions are thus irrelevant in the sequel. [If some density-density interaction is added here for the bosons, then the effective model (26) has to include it.]

We define the full Hamiltonian (fermion-boson compound system) by the symmetric operator

$$\mathbf{H} := H_f + H_b + W \in \mathcal{L}(\mathcal{D}, \mathcal{F}_{-,+}) , \quad (4)$$

where  $\mathcal{L}(\mathcal{D}, \mathcal{F}_{-,+})$  stands for the space of linear operators from  $\mathcal{D}$  to  $\mathcal{F}_{-,+}$  and

$$W := \sum_{x,y \in \mathbb{Z}^2} v(x-y) (b_x^* c_y + c_y^* b_x) \quad (5)$$

encodes (spin-conserving) exchange interactions between electron pairs and bipolarons (cf. Assumption 7) with  $\mathbb{Z}^2$ -summable coupling functions  $v$ . The fermionic operator  $c_x$  is defined, for all  $x \in \mathbb{Z}^2$  and some (large) parameter  $\kappa > 0$ , by

$$c_x := \sum_{z \in \mathbb{Z}^2, |z| \leq 1} e^{-\kappa|z|} a_{x+z, \uparrow} a_{x, \downarrow} . \quad (6)$$

Observe that the fermion–boson coupling is completely different from the one used in the celebrated Fröhlich model. For instance, in contrast to the Fröhlich model, it does not conserve the fermion number. Note also that we do not use the operator

$$\tilde{c}_x := \sum_{z \in \mathbb{Z}^2} e^{-\kappa|z|} a_{x+z, \uparrow} a_{x, \downarrow} = c_x + \mathcal{O}(e^{-\sqrt{2}\kappa}) \quad (7)$$

instead of  $c_x$  in the sequel in order to simplify technical arguments, only. The action of  $\tilde{c}_x$  can be viewed as the annihilation of an electron pair localized in a region of radius  $\mathcal{O}(\kappa^{-1})$ . It could be interesting to replace the Hubbard repulsion by general density–density interaction resulting from the second quantization of two–body interactions, like for instance

$$U \sum_{s \in \{\uparrow, \downarrow\}, x, y \in \mathbb{Z}^2} u(|x-y|) a_y^* a_y a_x^* a_x \quad (8)$$

on  $\mathcal{D}$ , where  $u(r) : \mathbb{R}_0^+ \rightarrow \mathbb{R}^+$  is some real-valued function. See discussion at the end of Section 3.2.

We consider fermion–boson interactions (5) with real-valued coupling functions  $v$  which are  $\mathbb{Z}^2$ -summable, symmetric and  $90^\circ$ -rotation invariant (cf. Assumption 9):  $v \in \ell^1(\mathbb{Z}^2, \mathbb{R})$  and, for all  $x \equiv (x_1, x_2) \in \mathbb{Z}^2$ ,

$$v(x) = v(-x) , \quad v(x) \equiv v(x_1, x_2) = v(-x_2, x_1) .$$

Note that the Fourier transform  $\hat{v}$  of such a  $v$  exists as a real-valued continuous function which is symmetric and  $90^\circ$ -rotation invariant, i.e., for all  $k \equiv (k_1, k_2) \in [-\pi, \pi]^2$ ,

$$\hat{v}(k) = \hat{v}(-k) , \quad \hat{v}(k) \equiv \hat{v}(k_1, k_2) = \hat{v}(-k_2, k_1) . \quad (9)$$

It is convenient, for reasons which become clear later on, to take  $v$  of the form

$$v = v_+ - v_- , \quad (10)$$

where  $v_{\pm} \in \ell^1(\mathbb{Z}^2, \mathbb{R})$  are functions of positive type, i.e., their Fourier transforms  $\hat{v}_{\pm}$  are non-negative.

### 3.2 $d$ -Wave Pairing in the 2-Fermions-1-Boson Sector

We aim to study the unitary group generated by  $\mathbf{H}$  on the smallest invariant space of  $\mathbf{H}$  containing the subspace related to one pair of electrons with total spin equal to zero. This invariant space is

$$\mathcal{H}_{\uparrow,\downarrow}^{(2,1)} := (\mathfrak{h}_{2,-}^{(0)} \otimes \mathfrak{h}_{0,+}) \oplus (\mathfrak{h}_{0,-} \otimes \mathfrak{h}_{1,+}) \simeq \mathfrak{h}_{2,-}^{(0)} \oplus \mathfrak{h}_{1,+} \quad (11)$$

with  $\mathfrak{h}_{2,-}^{(0)}$  being the subspace of one zero-spin fermion pair.  $\mathfrak{h}_{2,-}^{(0)}$  is canonically isomorphic to the spaces

$$\ell^2(\mathbb{Z}^2; \mathbb{C}) \otimes \ell^2(\mathbb{Z}^2; \mathbb{C}) \simeq \ell^2(\mathbb{Z}^2 \times \mathbb{Z}^2; \mathbb{C}) . \quad (12)$$

The first Hilbert space  $\ell^2(\mathbb{Z}^2; \mathbb{C})$  in the tensor product encodes the wave functions of a fermion with spin up ( $\uparrow$ ), whereas the second one refers to a fermion with spin down ( $\downarrow$ ). The isomorphism between  $\mathfrak{h}_{2,-}^{(0)}$  and  $\ell^2(\mathbb{Z}^2 \times \mathbb{Z}^2; \mathbb{C})$  is chosen in such a way that, for any  $x, y \in \mathbb{Z}^2$ ,  $a_{x,\uparrow}a_{y,\downarrow}$ , seen as an operator from  $\ell^2(\mathbb{Z}^2 \times \mathbb{Z}^2; \mathbb{C})$  to  $\mathbb{C}$ , satisfies

$$a_{x,\uparrow}a_{y,\downarrow}(\mathfrak{c}) = \mathfrak{c}(x, y) , \quad \mathfrak{c} \in \ell^2(\mathbb{Z}^2 \times \mathbb{Z}^2; \mathbb{C}) . \quad (13)$$

Since  $\mathfrak{h}_{1,+} = \ell^2(\mathbb{Z}^2; \mathbb{C})$ , it follows that

$$\mathcal{H}_{\uparrow,\downarrow}^{(2,1)} \simeq \ell^2(\mathbb{Z}^2 \times \mathbb{Z}^2; \mathbb{C}) \times \ell^2(\mathbb{Z}^2; \mathbb{C}) . \quad (14)$$

In particular, we denote elements  $\psi$  of  $\mathcal{H}_{\uparrow,\downarrow}^{(2,1)}$  by  $\psi = (\mathfrak{c}, \mathfrak{b})$ , where  $\mathfrak{c}$  and  $\mathfrak{b}$  are respectively the wave function of one fermion pair and one boson. Observe that

$$H^{(2,1)} := \overline{\mathbf{H}|_{\mathcal{H}_{\uparrow,\downarrow}^{(2,1)}}} \quad (15)$$

is a bounded self-adjoint operator on the subspace  $\mathcal{H}_{\uparrow,\downarrow}^{(2,1)}$ . Recall that  $v \in \ell^1(\mathbb{Z}^2, \mathbb{R})$ . We study below the unitary group generated by the Hamiltonian  $H^{(2,1)}$  in order to show the formation of a bound fermion pair of minimum energy via a mediating bipolaron (spinless boson, in the present case), as discussed in the introduction.

To this end, we define the ground state energy of the Hamiltonian  $H^{(2,1)}$  by

$$E_0 := \inf \sigma(H^{(2,1)}) ,$$

where  $\sigma(A)$  is, by definition, the spectrum of any self-adjoint operator  $A$ . From Lemma 8, observe that  $E_0 \leq 0$ . In fact, we can give an explicit criterium for the strict negativity of  $E_0$ , which is interpreted as a *bound fermion pair* formation. See Theorem 3 and discussion thereafter.

Indeed, for any  $\epsilon \geq 0$ ,  $\kappa > 0$ ,  $\lambda < 0$  and  $k \in [-\pi, \pi)^2$ , let

$$R_{s,s}^{(0)} := \frac{1}{(2\pi)^2} \int_{[-\pi,\pi)^2} \frac{1}{\epsilon(4 - \cos(k_{\uparrow\downarrow} - k) - \cos(k_{\uparrow\downarrow})) - \lambda} d^2 k_{\uparrow\downarrow} , \quad (16)$$

$$R_{d,d}^{(0)} := \frac{1}{(2\pi)^2} \int_{[-\pi,\pi)^2} \frac{(1 + 2e^{-\kappa} \cos(k_{\uparrow\downarrow} - k))^2}{\epsilon(4 - \cos(k_{\uparrow\downarrow} - k) - \cos(k_{\uparrow\downarrow})) - \lambda} d^2 k_{\uparrow\downarrow} , \quad (17)$$

$$R_{s,d}^{(0)} := \frac{1}{(2\pi)^2} \int_{[-\pi,\pi)^2} \frac{1 + 2e^{-\kappa} \cos(k_{\uparrow\downarrow} - k)}{\epsilon(4 - \cos(k_{\uparrow\downarrow} - k) - \cos(k_{\uparrow\downarrow})) - \lambda} d^2 k_{\uparrow\downarrow} , \quad (18)$$

where

$$\cos(q) := \cos(q_x) + \cos(q_y) , \quad q \equiv (q_x, q_y) \in [-\pi, \pi)^2 . \quad (19)$$

These strictly positive constants can easily be determined to a very high precision by numerical computations. Then, define the (possibly infinite) numbers

$$\begin{aligned} I(k, U) &:= \limsup_{\lambda \rightarrow 0^-} |\hat{v}(k)|^2 \left\{ \frac{R_{d,d}^{(0)}}{1 + UR_{s,s}^{(0)}} + U \frac{R_{d,d}^{(0)} R_{s,s}^{(0)} - (R_{s,d}^{(0)})^2}{1 + UR_{s,s}^{(0)}} \right\} \in [0, \infty] \\ I(k, \infty) &:= \limsup_{\lambda \rightarrow 0^-} |\hat{v}(k)|^2 \left\{ \frac{R_{d,d}^{(0)} R_{s,s}^{(0)} - (R_{s,d}^{(0)})^2}{R_{s,s}^{(0)}} \right\} \in [0, \infty] \end{aligned}$$

for any  $U \geq 0$  and  $k \in [-\pi, \pi)^2$ , see (64). A sufficient condition to obtain a bound pair (i.e.,  $E_0 < 0$ ) is as follows:

**Theorem 2 (Strict negativity of  $E_0$ )**

(i)  $E_0 < 0$  if and only if

$$\sup_{k \in [-\pi, \pi)^2} \{I(k, U) - \epsilon h_b(2 - \cos(k))\} > 0 .$$

The latter always holds true whenever  $\hat{v}(0) \neq 0$ .

(ii) At fixed  $\epsilon \geq 0$ ,

$$\liminf_{U \rightarrow \infty} E_0 < 0$$

if and only if

$$\sup_{k \in [-\pi, \pi]^2} \{I(k, \infty) - \epsilon h_b(2 - \cos(k))\} > 0 .$$

*Proof.* The assertions are direct consequences of Proposition 10 and Lemmata 11, 14 and 15.  $\square$

Note that Theorem 2 yields  $E_0 < 0$  for sufficiently small  $\epsilon \geq 0$ , unless  $v = 0$ .

We are interested in the time evolution driven by this Hamiltonian for three-body wave functions with minimum energy. We thus consider initial wave functions  $(\mathbf{c}_0, \mathbf{b}_0)$  in the subspace

$$\mathfrak{H}_\varepsilon := \text{Ran} \left( \mathbf{1}_{[E_0, E_0(1-\varepsilon)]}(H^{(2,1)}) \right) \subset \mathcal{H}_{\uparrow, \downarrow}^{(2,1)} \quad (20)$$

for small  $\varepsilon > 0$ . Here, for any  $\alpha_1, \alpha_2 \in \mathbb{R}$ ,  $\alpha_1 < \alpha_2$ , and self-adjoint operator  $A$ ,  $\mathbf{1}_{[\alpha_1, \alpha_2]}(A)$  denotes the spectral projector of  $A$  associated to its spectrum in the interval  $[\alpha_1, \alpha_2]$ , while  $\text{Ran}(A)$  stands for the range of  $A$ . Note that  $E_0$  is generally not an eigenvalue of  $H^{(2,1)}$ , see Section 5.

Then, for any positive real number  $0 < \varepsilon \ll 1$ , we study the properties of the time-dependent wave function  $(\mathbf{c}_t, \mathbf{b}_t)$ , solution of the Schrödinger equation

$$\forall t \in \mathbb{R} : i \frac{d}{dt}(\mathbf{c}_t, \mathbf{b}_t) = H^{(2,1)}(\mathbf{c}_t, \mathbf{b}_t) , \quad (\mathbf{c}_t, \mathbf{b}_t) \in \mathfrak{H}_\varepsilon . \quad (21)$$

With this aim, define the (non-empty) set

$$\Xi_\varepsilon := \left\{ (\mathbf{c}_t, \mathbf{b}_t) \in C^1(\mathbb{R}, \mathfrak{H}_\varepsilon) \text{ norm-one solution of Equation (21)} \right\}$$

for  $0 < \varepsilon \ll 1$ . Units are chosen so that  $\hbar = 1$ .

We first show that the strict negativity of  $E_0$  corresponds to the existence a bound fermion pair:

**Theorem 3 (Existence of bound fermion pairs)**

Assume that  $E_0 < 0$ . For any  $\eta, \varepsilon \in (0, 1)$  and  $(\mathbf{c}_t, \mathbf{b}_t) \in \Xi_\varepsilon$ , there is a constant  $R < \infty$  such that, for all  $t \in \mathbb{R}$ ,

$$\sum_{x_\uparrow, x_\downarrow \in \mathbb{Z}^2 : |x_\uparrow - x_\downarrow| \leq R} |\mathbf{c}_t(x_\uparrow, x_\downarrow)|^2 \geq \|\mathbf{c}_0\|_2^2 (1 - \eta) > 0 .$$

Moreover, if the hopping amplitude  $\epsilon > 0$  is sufficiently small then one can choose  $R = 1$ .

*Proof.* It is a direct consequence of Proposition 13.  $\square$

Since  $(\mathbf{c}_t, \mathbf{b}_t) \in \Xi_\varepsilon$  has norm one for all  $t \in \mathbb{R}$ , we infer from Theorem 3 that, uniformly in time  $t$ , the probability of finding an electron pair in a region of diameter 1 is always strictly positive for strictly negative  $E_0 < 0$  and sufficiently small hopping amplitude  $0 \leq \varepsilon \ll 1$ . In other words, the fermion part  $\mathbf{c}_t$  never vanishes in this regime while the two fermions behave as a composite particle, i.e., a bound fermion pair. We also have a non-vanishing boson part  $\mathbf{b}_t$  for all times. The latter can be seen as a depletion of either the pair density or the boson (bipolaron) density. This depletion results from the interaction  $W$  (5) which implies an effective attraction between fermions. This can heuristically be understood by diagrammatic methods like in [17]. It is also reminiscent of the Bose condensate depletion found in the rigorous study of the Bogoliubov model and its variants. See for instance [18, 19]. The boson-fermion occupation ratio can be explicitly computed in the limits  $\varepsilon \rightarrow 0$  and  $U \rightarrow \infty$ :

$$\frac{\|\mathbf{c}_t\|_2^2}{\|\mathbf{c}_t\|_2^2 + \|\mathbf{b}_t\|_2^2} \rightarrow \frac{1}{2} \quad (22)$$

see Lemma 23. Similar results in the regime  $\varepsilon \rightarrow 0$  and  $U \rightarrow 0$  can also be deduced from our study.

For sufficiently small hopping amplitudes, the last theorem says that the bound pair is (s) either localized on a single lattice site or (d) the fermions forming the bound pair have distance exactly equal to 1 to each other. (s) mainly appears at small coupling  $U \geq 0$  and corresponds to a  $s$ -wave pair. By contrast, (d) occurs at large  $U \geq 0$  and is related to the formation of a  $d$ -wave pair whenever Assumption 7 is satisfied. If this assumption does not hold, we still have, at large  $U \geq 0$ , a distance exactly equal to 1 between the fermions in the bound pair, but the pairing symmetry is rather of *generalized*  $s$ -wave type instead of  $d$ -wave. We now devote the rest of this section to the precise statements of these facts.

At any  $k \in [-\pi, \pi)^2$ , define the function  $\mathbf{s}_k : \mathbb{Z}^2 \rightarrow \mathbb{C}$  by

$$\mathbf{s}_k(y) := \frac{1}{2} \left( e^{ik \cdot (0,1)} \delta_{y,(0,1)} + e^{ik \cdot (0,-1)} \delta_{y,(0,-1)} + e^{ik \cdot (1,0)} \delta_{y,(1,0)} + e^{ik \cdot (-1,0)} \delta_{y,(-1,0)} \right) \quad (23)$$

for all  $y \in \mathbb{Z}^2$ . Let

$$\mathfrak{K}_v := \left\{ k \in [-\pi, \pi)^2 : |\hat{v}(k)| = \max_{q \in [-\pi, \pi)^2} |\hat{v}(q)| =: \|\hat{v}\|_\infty \right\} \quad (24)$$

be the non-empty closed set of maximizers of the absolute value of the Fourier transform  $\hat{v}$  of  $v \in \ell^1(\mathbb{Z}^2, \mathbb{R})$ .

**Theorem 4 (Generic space symmetry of bound pairs)**

Assume that  $\mathfrak{K}_v$  is a finite set and take any  $\eta > 0$ . For sufficiently small  $\varepsilon, \epsilon > 0$  and any  $(\mathfrak{c}_t, \mathfrak{b}_t) \in \Xi_\varepsilon$ , there is a family  $\{f^{(k)}\}_{k \in \mathfrak{K}} \subset C(\mathbb{R}, \ell^2(\mathbb{Z}^2; \mathbb{C}))$  of one-particle wave functions such that:

(s) For sufficiently small  $U \geq 0$  and all  $t \in \mathbb{R}$ ,

$$\sum_{x_\uparrow, x_\downarrow \in \mathbb{Z}^2} \left| \mathfrak{c}_t(x_\uparrow, x_\downarrow) - \sum_{k \in \mathfrak{K}_v} \{ \delta_{x_\uparrow, x_\downarrow} + 2e^{-\kappa} \mathfrak{s}_k(x_\uparrow - x_\downarrow) \} f_t^{(k)}(x_\uparrow) \right|^2 \leq \eta.$$

(d) For sufficiently large  $U > 0$  and all  $t \in \mathbb{R}$ ,

$$\sum_{x_\uparrow, x_\downarrow \in \mathbb{Z}^2} \left| \mathfrak{c}_t(x_\uparrow, x_\downarrow) - \sum_{k \in \mathfrak{K}_v} \mathfrak{s}_k(x_\uparrow - x_\downarrow) f_t^{(k)}(x_\uparrow) \right|^2 \leq \eta.$$

*Proof.* It is a direct consequence of Corollaries 17–18, Proposition 21 and Lemma 22. Note that Proposition 21 only treats the case of large  $U \gg 1$  and Lemma 22 analyzes the  $\mathfrak{d}$ -component of the wave function. To get Assertion (s) we need similar results for the  $\mathfrak{s}$ -component at small  $U \ll 1$ . We omit the details since the latter case is even simpler.  $\square$

If the above theorem holds and  $\hat{v}$  is concentrated on half breathing bond-stretching modes, i.e.,

$$\mathfrak{K}_v = \{(-\pi, 0), (0, -\pi)\} \subset [-\pi, \pi]^2 \quad (25)$$

(cf. Assumption 7), then the system shows  $d$ -wave pairing:

**Corollary 5 ( $d$ -wave space symmetry)**

Assume (25) and take  $\eta > 0$ . For sufficiently small  $\varepsilon, \epsilon > 0$  and any  $(\mathfrak{c}_t, \mathfrak{b}_t) \in \Xi_\varepsilon$ , there is a one-particle wave function  $f_\varepsilon \in C(\mathbb{R}, \ell^2(\mathbb{Z}^2; \mathbb{C}))$  such that, for sufficiently large  $U > 0$  and all  $t \in \mathbb{R}$ ,

$$\sum_{x_\uparrow, x_\downarrow \in \mathbb{Z}^2} \left| \mathfrak{c}_t(x_\uparrow, x_\downarrow) - \mathfrak{d}(x_\uparrow - x_\downarrow) f_t(x_\uparrow) \right|^2 \leq \eta,$$

where

$$\mathfrak{d} := \mathfrak{s}_{(-\pi, 0)} = -\mathfrak{s}_{(0, -\pi)}.$$



If  $|\hat{v}(\pm\pi, 0)|$  (or  $|\hat{v}(0, \pm\pi)|$ ) is sufficiently large, then the wave function of the bound fermion pair has the  $d$ -wave symmetry, by Corollary 5. Indeed, the Fourier transform  $\hat{\mathbf{d}}$  of  $\mathbf{d}$  equals

$$\hat{\mathbf{d}}(k) \equiv \hat{\mathbf{d}}(k_1, k_2) = \cos(k_2) - \cos(k_1)$$

for any  $k \equiv (k_1, k_2) \in [-\pi, \pi)^2$ . [See for instance (89).] This is precisely the orbital function of the  $d$ -wave pair configuration, see [1].

Note that the Hubbard repulsion could be replaced by a general density-density interaction resulting from the second quantization of two-body interactions, like for instance (8). In this case, one has to consider the more general fermion pair annihilation operator  $\tilde{c}_x$  as given by (7) (instead of  $c_x$ ). Such models would lead to much more general pairing configurations, beyond  $s$ - and  $d$ -wave orbitals. Basically, if  $u(r)$  has finite range  $[0, R]$  then in the limit  $U \rightarrow \infty$  bound fermion pairs of radius less than  $R$  will be suppressed, but the interaction  $W$  will bind pairs of fermion separated by a distance of at least  $R$ , even when  $U \rightarrow \infty$ . In this case, the minimum energy of the system does not depend much on  $U$ . Similar methods to those used here should be applicable to such a more general situation. However, we only consider the most simple physically relevant case  $R = 0$  to keep technical aspects as simple as possible.

## 4 Uncoupled Effective Models for High- $T_c$ Superconductors

### 4.1 Definition of the Effective Model

We propose a model which decouples bosons and fermions but which correctly describes the dynamics of the original model at low energies within the invariant space  $\mathcal{H}_{\uparrow, \downarrow}^{(2,1)}$ , as described in Section 3.2. The fermionic part is a BCS-like model, as usually done in theoretical physics, while the bosonic part is a free model with effective hopping amplitudes.

Indeed, using the decomposition (10) we define the bosonic effective Hamiltonian on the dense subspace  $\mathcal{D}(1)$  by the symmetric operator

$$\tilde{H}_b := - \sum_{x, y \in \mathbb{Z}^2, |x-y|=1} w_b(x-y) b_x^* b_y \quad (26)$$

with

$$w_b(x) := \gamma_b(v_+(x) + v_-(x)) + \frac{1}{2U}(v * v)(x), \quad x \in \mathbb{Z}^2, \quad (27)$$

and  $\gamma_b \geq 0$ . Note that the function  $w_b \in \ell^1(\mathbb{Z}^2, \mathbb{R})$  is of positive type, and hence the bosonic hopping amplitudes are of negative type.  $w_b$  is however not necessarily positive, as usual hopping terms. Meanwhile, the fermionic effective Hamiltonian is defined on  $\mathcal{D}$  by the symmetric operator

$$\begin{aligned} \tilde{H}_f := & \epsilon \left( -\frac{1}{2} \sum_{s \in \{\uparrow, \downarrow\}, x, y \in \mathbb{Z}^2, |x-y|=1} a_{x,s}^* a_{y,s} + 2 \sum_{s \in \{\uparrow, \downarrow\}, x \in \mathbb{Z}^2} a_{x,s}^* a_{x,s} \right) \\ & + U \sum_{x \in \mathbb{Z}^2} n_{x,\uparrow} n_{x,\downarrow} - \sum_{x, y \in \mathbb{Z}^2} w_f(x-y) c_x^* c_y \end{aligned} \quad (28)$$

with

$$w_f(x) := \gamma_f(v_+(x) + v_-(x)) - \frac{\gamma_f^2}{2U+1}(v * v)(x), \quad x \in \mathbb{Z}^2, \quad (29)$$

and  $\epsilon, U, \gamma_f \geq 0$ . See (6) for the definition of  $c_x$ . Observe that, at large enough  $U > 0$ , the BCS-like kernel above is of negative type and is thus of *attractive* nature. The precise form (29) we have chosen for  $w_f$  is obtained by imposing that the effective model gives the exact energy and fermionic wave-function at orders  $U^0$  and  $U^{-1}$ , by expanding these quantities at any fixed quasi-momentum. Recall that we focus on the large- $U$  regime, because this is the one related to  $d$ -wave pairing.

Then, the uncoupled effective model is defined by

$$\tilde{\mathbf{H}} := \tilde{H}_f + \tilde{H}_b \in \mathcal{L}(\mathcal{D}, \mathcal{F}_{-,+}). \quad (30)$$

Because of (9), the uncoupled model is  $90^\circ$ -rotation, reflection and translation invariant, in accordance to Assumption 9.

As in the case of the boson-fermion model  $\mathbf{H}$ , the subspace  $\mathcal{H}_{\uparrow, \downarrow}^{(2,1)}$  is an invariant space of  $\tilde{\mathbf{H}}$ . Therefore, we analyze the dynamics driven by the bounded self-adjoint operator

$$\tilde{H}^{(2,1)} := \overline{\tilde{\mathbf{H}}|_{\mathcal{H}_{\uparrow, \downarrow}^{(2,1)}}}$$

at the bottom of its spectrum in order to compare it with the one given by  $H^{(2,1)}$ , see (15) and (21). The result is the following:

**Theorem 6 (Effectiveness of the uncoupled model)**

Set  $\gamma_b := 2e^{-\kappa}$  and  $\gamma_f = \gamma_b^{-1}$ . Then, there is  $\varepsilon_0 > 0$  such that, uniformly for  $\varepsilon \in (0, \varepsilon_0)$ ,  $t \in \mathbb{R}$ , and  $\epsilon, U > 0$ ,

$$\left\| \left( e^{-itH^{(2,1)}} - e^{-it\tilde{H}^{(2,1)}} \right) \mathbf{1}_{[E_0, E_0(1-\varepsilon)]}(H^{(2,1)}) \right\|_{\text{op}} = \mathcal{O}((1 + |t|)(\epsilon + U^{-2})) .$$

*Proof.* The proof is a direct consequence of Lemmata 7 and 20, Corollary 18, Equations (90)–(91), and Propositions 24–25.  $\square$

If the functions  $v_{\pm}$  decay sufficiently fast in space, then we can find kernels  $w_b, w_f \in \ell^1(\mathbb{Z}^2, \mathbb{R})$  of positive type such that

$$\left\| \left( e^{-itH^{(2,1)}} - e^{-it\tilde{H}^{(2,1)}} \right) \mathbf{1}_{[E_0, E_0(1-\varepsilon)]}(H^{(2,1)}) \right\|_{\text{op}} = \mathcal{O}(\epsilon + U^{-2}) ,$$

uniformly in time  $t \in \mathbb{R}$ . Indeed, when  $E_0 < 0$ , one chooses  $w_f$  and  $w_b$  with Fourier transform  $\hat{w}_f$  and  $\hat{w}_b$ , respectively, such that

$$\hat{w}_f(k) \mathcal{R}(k, U, E(k)) = 1$$

and  $\hat{w}_b(k) = E(k)$  for  $k$  in open neighborhood of the set of minimizers of  $E(\cdot)$  on  $[-\pi, \pi]^2$ . See Proposition 10, Theorem 12, and Equation (92).

## 4.2 Long–Range Idealization of the Effective Electron–Electron Interaction

The analysis of equilibrium states of fermionic models like (28) is known to be a very difficult task. Indeed, the complete phase diagram of the Hubbard model, which is (28) with  $w_f \equiv 0$ , is still unknown for dimensions bigger than one, at least in a mathematically rigorous sense. However, for certain classes of long–range couplings  $w_f$ , the equilibrium states of (28) become much more tractable: We showed in [20] how to construct equilibrium states of long–range models as convex combinations of equilibrium states of much more simple “Bogolioubov approximations” of the starting model.

By Assumption 7, the Fourier transform  $\hat{v}$  of the coupling function  $v$  is concentrated around a few points in the Brillouin zone. See (25). This implies from (29) that  $\hat{w}_f$  is also concentrated around the same points. We can thus consider the idealization where the Fourier transform  $\hat{w}_f$  tends to a distribution supported on that few points. More precisely, it is reasonable to replace  $\hat{w}_f$  by

$$w_f^{(\text{MF})}(x) := \gamma_f^{(\text{MF})} \left( e^{i(-\pi, 0) \cdot x} + e^{i(0, -\pi) \cdot x} \right)$$

for  $x \in \mathbb{Z}^2$ , where  $\gamma_f^{(\text{MF})} \geq 0$  is a positive constant. However, this kernel is not anymore summable in the  $\mathbb{Z}^2$ -lattice. The corresponding interaction has thus to be interpreted as a mean field term. Hence, we define the corresponding mean field type model in cubic boxes  $\Lambda_l \subset \mathbb{Z}^2$  of size length  $l \in \mathbb{R}^+$  with volume  $|\Lambda_l|$ :

$$\begin{aligned} \tilde{H}_{f,l}^{(\text{MF})} := & \epsilon \left( -\frac{1}{2} \sum_{s \in \{\uparrow, \downarrow\}, x, y \in \Lambda_l, |x-y|=1} a_{x,s}^* a_{y,s} + 2 \sum_{s \in \{\uparrow, \downarrow\}, x \in \Lambda_l} a_{x,s}^* a_{x,s} \right) \\ & + 2U \sum_{x \in \Lambda_l} n_{x,\uparrow} n_{x,\downarrow} - \frac{1}{|\Lambda_l|} \sum_{x, y \in \Lambda_l} w_f^{(\text{MF})}(x-y) c_x^* c_y. \end{aligned} \quad (31)$$

Compare with (28). Observe that the last term is  $|\Lambda_l|$  times the sum of the squares of the space averages of two operators:

$$\begin{aligned} & \frac{1}{|\Lambda_l|} \sum_{x, y \in \Lambda_l} w_f^{(\text{MF})}(x-y) c_x^* c_y \\ = & \gamma^{(\text{MF})} |\Lambda_l| \left( \frac{1}{|\Lambda_l|} \sum_{x \in \Lambda_l} e^{i(\pi, 0) \cdot x} c_x \right)^* \left( \frac{1}{|\Lambda_l|} \sum_{x \in \Lambda_l} e^{i(\pi, 0) \cdot x} c_x \right) \\ & + \gamma^{(\text{MF})} |\Lambda_l| \left( \frac{1}{|\Lambda_l|} \sum_{x \in \Lambda_l} e^{i(0, \pi) \cdot x} c_x \right)^* \left( \frac{1}{|\Lambda_l|} \sum_{x \in \Lambda_l} e^{i(0, \pi) \cdot x} c_x \right). \end{aligned}$$

This leads to a long-range interaction (cf. Assumption 8) similar to the ones treated in [20]. The long-range component of the model discussed here is rather a sum over periodic (but not translation invariant) mean field type quadratic terms. The methods of [20] have to be adapted to this case, but they are still applicable.

In this case, one has to be able to study the “Bogolioubov approximations” of the model  $\tilde{H}_{f,l}^{(\text{MF})}$ , at least in the strong coupling regime (Cf. Assumption 2), i.e., for  $\epsilon = 0$ . It is also important to check that the behavior of the system is not singular at  $\epsilon = 0$ . In this context, methods of constructive quantum field theory, as Grassmann–Berezin integrations, Brydges–Kennedy tree expansions and determinant bounds [21] will be important. We recently applied such methods in a similar situation in [22] to analyze the Meissner–Ochsenfeld effect, starting from a microscopic model. Technically speaking, this last study is difficult. We plan to work out these problems in subsequent papers.

## 5 Technical Proofs

Before starting, note that the computations are given in all details to make them “self-contained” and hence accessible to readers not used with the methods. Even if it is not explicitly mentioned, we always have  $\epsilon, U, h_b \geq 0$  and  $\kappa > 0$ . For simplicity and without loss of generality, in this section we sometimes fix  $h_b \in [0, 1]$ .

### 5.1 Fiber Decomposition of the 2-Fermions–1-Boson Hamiltonian

The (fermionic and bosonic) kinetic parts of the Hamiltonian  $H^{(2,1)}$  defined by (15) are diagonalizable by the Fourier transform. The interaction term (5) is such that it annihilates either a boson to create a fermion pair or a fermion pair to create a boson with same total quasi-momentum, in both cases. As a consequence, it is natural to decompose  $H^{(2,1)}$  on fibers parametrized by Fourier modes  $k \in [-\pi, \pi]^2$ , which stand for total quasi-momenta on the torus. It is done as follows:

We denote the Haar measure on the torus  $[-\pi, \pi]^2$  by  $\mathfrak{m}$ , i.e.,

$$\mathfrak{m}(d^2q) := (2\pi)^{-2} d^2q .$$

Using the direct integral of Hilbert spaces (see Section 6.1), let

$$\begin{aligned} \mathfrak{F}_{\uparrow, \downarrow}^{(2,1)} &:= \int_{[-\pi, \pi]^2}^{\oplus} L^2([-\pi, \pi]^2, \mathfrak{m}; \mathbb{C}) \times \mathbb{C} \mathfrak{m}(d^2k) \\ &\simeq \int_{[-\pi, \pi]^2}^{\oplus} L^2([-\pi, \pi]^2, \mathfrak{m}; \mathbb{C}) \mathfrak{m}(d^2k) \times L^2([-\pi, \pi]^2, \mathfrak{m}; \mathbb{C}) . \end{aligned}$$

This space is also unitarily equivalent to the Hilbert space

$$\mathcal{H}_{\uparrow, \downarrow}^{(2,1)} \simeq \ell^2(\mathbb{Z}^2 \times \mathbb{Z}^2; \mathbb{C}) \times \ell^2(\mathbb{Z}^2; \mathbb{C}) ,$$

see (11) and (14). An isometry between both spaces is defined by

$$\mathfrak{U}(\hat{\mathbf{c}}, \hat{\mathbf{b}}) := (\mathfrak{U}_{\uparrow, \downarrow}(\hat{\mathbf{c}}), \mathfrak{U}_b(\hat{\mathbf{b}})) \in \mathcal{H}_{\uparrow, \downarrow}^{(2,1)} , \quad (\hat{\mathbf{c}}, \hat{\mathbf{b}}) \in \mathfrak{F}_{\uparrow, \downarrow}^{(2,1)} , \quad (32)$$

where the wave function  $\mathfrak{U}_{\uparrow, \downarrow}(\hat{\mathbf{c}})$  of one fermion pair in  $\mathcal{H}_{\uparrow, \downarrow}^{(2,1)}$  equals

$$\begin{aligned} [\mathfrak{U}_{\uparrow, \downarrow}(\hat{\mathbf{c}})](x_{\uparrow}, x_{\downarrow}) &:= \int_{[-\pi, \pi]^2} \mathfrak{m}(d^2k) \int_{[-\pi, \pi]^2} \mathfrak{m}(d^2k_{\uparrow, \downarrow}) \\ &\quad e^{ik \cdot x_{\uparrow}} e^{ik_{\uparrow, \downarrow} \cdot (x_{\downarrow} - x_{\uparrow})} [\hat{\mathbf{c}}(k)](k_{\uparrow, \downarrow}) , \end{aligned} \quad (33)$$

for any  $x_\uparrow, x_\downarrow \in \mathbb{Z}^2$ , while the wave function  $\mathfrak{U}_b(\hat{\mathfrak{b}})$  of one boson is

$$[\mathfrak{U}_b(\hat{\mathfrak{b}})](x_b) := \int_{[-\pi, \pi]^2} e^{ik \cdot x_b} \hat{\mathfrak{b}}(k) \, \mathfrak{m}(d^2 k) \quad (34)$$

for  $x_b \in \mathbb{Z}^2$ . Since

$$L^2([-\pi, \pi]^2 \times [-\pi, \pi]^2, \mathfrak{m} \otimes \mathfrak{m}; \mathbb{C}) \subset L^1([-\pi, \pi]^2 \times [-\pi, \pi]^2, \mathfrak{m} \otimes \mathfrak{m}; \mathbb{C}) , \quad (35)$$

and

$$L^2([-\pi, \pi]^2, \mathfrak{m}; \mathbb{C}) \subset L^1([-\pi, \pi]^2, \mathfrak{m}; \mathbb{C}) , \quad (36)$$

note that the r.h.s. of (33)–(34) are well-defined. Moreover, the operators

$$\mathfrak{U}_{\uparrow\downarrow} : \int_{[-\pi, \pi]^2}^{\oplus} L^2([-\pi, \pi]^2, \mathfrak{m}; \mathbb{C}) \, \mathfrak{m}(d^2 k) \rightarrow \ell^2(\mathbb{Z}^2 \times \mathbb{Z}^2; \mathbb{C})$$

and

$$\mathfrak{U}_b : L^2([-\pi, \pi]^2, \mathfrak{m}; \mathbb{C}) \rightarrow \ell^2(\mathbb{Z}^2; \mathbb{C})$$

are unitary. The inverse  $\mathfrak{U}^{-1} = \mathfrak{U}^*$  is

$$\mathfrak{U}^* = \mathfrak{U}_{\uparrow\downarrow}^* \oplus \mathfrak{U}_b^* \quad (37)$$

and  $\mathfrak{F}_{\uparrow\downarrow}^{(2,1)} = \mathfrak{U}^* \mathcal{H}_{\uparrow\downarrow}^{(2,1)}$  (using (14)).

To obtain explicit expressions for the actions of  $\mathfrak{U}_{\uparrow\downarrow}^*$  and  $\mathfrak{U}_b^*$ , it suffices to consider dense subspaces of  $\ell^2(\mathbb{Z}^2 \times \mathbb{Z}^2; \mathbb{C})$  and  $\ell^2(\mathbb{Z}^2; \mathbb{C})$ , respectively. Note indeed that, in contrast with (35)–(36),

$$\ell^1(\mathbb{Z}^2 \times \mathbb{Z}^2; \mathbb{C}) \subsetneq \ell^2(\mathbb{Z}^2 \times \mathbb{Z}^2; \mathbb{C}) \quad \text{and} \quad \ell^1(\mathbb{Z}^2; \mathbb{C}) \subsetneq \ell^2(\mathbb{Z}^2; \mathbb{C}) .$$

For any  $\mathfrak{c} \in \ell^1(\mathbb{Z}^2 \times \mathbb{Z}^2; \mathbb{C})$  and  $k, k_{\uparrow\downarrow} \in [-\pi, \pi]^2$ ,

$$[\mathfrak{U}_{\uparrow\downarrow}^*(\mathfrak{c})](k) = \sum_{x_\uparrow, x_{\uparrow\downarrow} \in \mathbb{Z}^2} e^{-ik \cdot x_\uparrow} e^{-ik_{\uparrow\downarrow} \cdot x_{\uparrow\downarrow}} \mathfrak{c}(x_\uparrow, x_\uparrow + x_{\uparrow\downarrow}) ,$$

while, for any  $\mathfrak{b} \in \ell^1(\mathbb{Z}^2; \mathbb{C})$  and  $k \in [-\pi, \pi]^2$ ,

$$\mathfrak{U}_b^*(\mathfrak{b})(k) = \sum_{x_b \in \mathbb{Z}^2} e^{-ik \cdot x_b} \mathfrak{b}(x_b) .$$

Now we study the operator  $\mathfrak{U}^* H^{(2,1)} \mathfrak{U}$  acting on  $\mathfrak{F}_{\uparrow,\downarrow}^{(2,1)}$  (cf. (15)). We start by deriving that its fiber decomposition (see Section 6.1 for more details). To this end, recall that  $\hat{v}$  is the Fourier transform of the coupling function  $v$  and, at each  $k \in [-\pi, \pi]^2$ , let  $\mathfrak{s}, \mathfrak{d}(k) \in L^2([-\pi, \pi]^2, \mathfrak{m}; \mathbb{C})$  be defined by

$$\mathfrak{s}(k_{\uparrow\downarrow}) := 1 \quad \text{and} \quad [\mathfrak{d}(k)](k_{\uparrow\downarrow}) := 2e^{-\kappa} \cos(k_{\uparrow\downarrow} - k) , \quad (38)$$

for all  $k_{\uparrow\downarrow} \in [-\pi, \pi]^2$ , where the function  $\cos$  is defined on the torus  $[-\pi, \pi]^2$  by (19). Let  $P_{\mathfrak{d}(k)} = P_{\mathfrak{d}(k)}^* \in \mathcal{B}(L^2([-\pi, \pi]^2, \mathfrak{m}; \mathbb{C}))$  be the orthogonal projection with range

$$\text{Ran}(P_{\mathfrak{d}(k)}) = \mathbb{C}(\mathfrak{d}(k) + \mathfrak{s}) . \quad (39)$$

Similarly,  $P_0 = P_0^* \in \mathcal{B}(L^2([-\pi, \pi]^2, \mathfrak{m}; \mathbb{C}))$  is the orthogonal projection with range

$$\text{Ran}(P_0) = \mathbb{C}\mathfrak{s} . \quad (40)$$

At any  $k \in [-\pi, \pi]^2$ , define now the bounded operators

$$\begin{aligned} A_{1,1}^{(0)}(k) &: L^2([-\pi, \pi]^2, \mathfrak{m}; \mathbb{C}) \rightarrow L^2([-\pi, \pi]^2, \mathfrak{m}; \mathbb{C}) , \\ A_{1,1}(k) &: L^2([-\pi, \pi]^2, \mathfrak{m}; \mathbb{C}) \rightarrow L^2([-\pi, \pi]^2, \mathfrak{m}; \mathbb{C}) , \\ A_{2,1}(k) &: L^2([-\pi, \pi]^2, \mathfrak{m}; \mathbb{C}) \rightarrow \mathbb{C} , \\ A_{1,2}(k) &: \mathbb{C} \rightarrow L^2([-\pi, \pi]^2, \mathfrak{m}; \mathbb{C}) , \\ A_{2,2}(k) &: \mathbb{C} \rightarrow \mathbb{C} , \end{aligned}$$

by

$$[A_{1,1}^{(0)}(k)\Psi_{\uparrow\downarrow}](k_{\uparrow\downarrow}) := \epsilon(4 - \cos(k_{\uparrow\downarrow} - k) - \cos(k_{\uparrow\downarrow})) \Psi_{\uparrow\downarrow}(k_{\uparrow\downarrow}) , \quad (41)$$

$$A_{1,1}(k)\Psi_{\uparrow\downarrow} := A_{1,1}^{(0)}(k)\Psi_{\uparrow\downarrow} + UP_0\Psi_{\uparrow\downarrow} , \quad (42)$$

$$A_{2,1}(k)\Psi_{\uparrow\downarrow} := \hat{v}(k) \langle \mathfrak{d}(k) + \mathfrak{s}, \Psi_{\uparrow\downarrow} \rangle , \quad (43)$$

$$A_{1,2}(k)\Psi_b := \Psi_b \hat{v}(k) (\mathfrak{d}(k) + \mathfrak{s}) , \quad (44)$$

$$A_{2,2}(k)\Psi_b := \epsilon h_b(2 - \cos(k))\Psi_b , \quad (45)$$

for all  $\Psi_{\uparrow\downarrow} \in L^2([-\pi, \pi]^2, \mathfrak{m}; \mathbb{C})$  and  $\Psi_b \in \mathbb{C}$ . Here,  $\langle \cdot, \cdot \rangle$  stands for the scalar product of  $L^2([-\pi, \pi]^2, \mathfrak{m}; \mathbb{C})$ . By continuity of  $\hat{v}$ , the maps  $k \mapsto A_{i,j}(k)$  are continuous, in operator norm sense, for all  $i, j \in \{1, 2\}$ . In particular,

$$A(\cdot) := \begin{pmatrix} A_{1,1}(\cdot) & A_{1,2}(\cdot) \\ A_{2,1}(\cdot) & A_{2,2}(\cdot) \end{pmatrix} \in L^\infty([-\pi, \pi]^2, \mathfrak{m}; \mathcal{B}(L^2([-\pi, \pi]^2, \mathfrak{m}; \mathbb{C}) \times \mathbb{C})) . \quad (46)$$

By [23, Theorem XIII.83] (see also Section 6.1), there is a unique decomposable operator

$$A := \int_{[-\pi, \pi)^2}^{\oplus} A(k) \, \mathfrak{m}(d^2 k) \in \mathcal{B}(\mathfrak{F}_{\uparrow, \downarrow}^{(2,1)}) , \quad (47)$$

which turns out to coincide with  $\mathfrak{U}^* H^{(2,1)} \mathfrak{U}$ :

**Lemma 7 (Direct integral decomposition)**

$$A = \mathfrak{U}^* H^{(2,1)} \mathfrak{U} \quad \text{and} \quad \|H^{(2,1)}\|_{\text{op}} = \max_{k \in [-\pi, \pi)^2} \|A(k)\|_{\text{op}} .$$

*Proof.* Define the dense set

$$\mathcal{D}_{\uparrow, \downarrow}^{(2,1)} := \mathfrak{U}^* [\ell^1(\mathbb{Z}^2 \times \mathbb{Z}^2; \mathbb{C}) \times \ell^1(\mathbb{Z}^2; \mathbb{C})] \subset \mathfrak{F}_{\uparrow, \downarrow}^{(2,1)} .$$

For any  $(\hat{\mathfrak{c}}, \hat{\mathfrak{b}}) \in \mathcal{D}_{\uparrow, \downarrow}^{(2,1)}$ , we infer from (2), (3), (4), (5), (6), and (13) that

$$H^{(2,1)} \mathfrak{U}(\hat{\mathfrak{c}}, \hat{\mathfrak{b}}) = (\mathfrak{c}', \mathfrak{b}') \in \mathcal{H}_{\uparrow, \downarrow}^{(2,1)} ,$$

where, for any  $x_{\uparrow}, x_{\downarrow} \in \mathbb{Z}^2$ ,

$$\begin{aligned} \mathfrak{c}'(x_{\uparrow}, x_{\downarrow}) &= -\frac{\epsilon}{2} \sum_{z \in \mathbb{Z}^2, |z|=1} [\mathfrak{U}_{\uparrow \downarrow}(\hat{\mathfrak{c}})](x_{\uparrow} + z, x_{\downarrow}) - \frac{\epsilon}{2} \sum_{z \in \mathbb{Z}^2, |z|=1} [\mathfrak{U}_{\uparrow \downarrow}(\hat{\mathfrak{c}})](x_{\uparrow}, x_{\downarrow} + z) \\ &\quad + 4\epsilon [\mathfrak{U}_{\uparrow \downarrow}(\hat{\mathfrak{c}})](x_{\uparrow}, x_{\downarrow}) + U \delta_{x_{\uparrow}, x_{\downarrow}} [\mathfrak{U}_{\uparrow \downarrow}(\hat{\mathfrak{c}})](x_{\uparrow}, x_{\downarrow}) \\ &\quad + \sum_{x_b \in \mathbb{Z}^2} v(x_{\downarrow} - x_b) \delta_{x_{\uparrow}, x_{\downarrow}} [\mathfrak{U}_b(\hat{\mathfrak{b}})](x_b) \\ &\quad + e^{-\kappa} \sum_{x_b \in \mathbb{Z}^2} \sum_{z \in \mathbb{Z}^2, |z|=1} v(x_{\downarrow} - x_b) \delta_{x_{\uparrow} + z, x_{\downarrow}} [\mathfrak{U}_b(\hat{\mathfrak{b}})](x_b) \end{aligned}$$

and, for any  $x_b \in \mathbb{Z}^2$ ,

$$\begin{aligned} \mathfrak{b}'(x_b) &= -\frac{\epsilon h_b}{2} \sum_{z \in \mathbb{Z}^2, |z|=1} [\mathfrak{U}_b(\hat{\mathfrak{b}})](x_b + z) + 2\epsilon h_b [\mathfrak{U}_b(\hat{\mathfrak{b}})](x_b) \\ &\quad + \sum_{x \in \mathbb{Z}^2} v(x_b - x) [\mathfrak{U}_{\uparrow \downarrow}(\hat{\mathfrak{c}})](x, x) \\ &\quad + e^{-\kappa} \sum_{x \in \mathbb{Z}^2} \sum_{z \in \mathbb{Z}^2, |z|=1} v(x_b - x) [\mathfrak{U}_{\uparrow \downarrow}(\hat{\mathfrak{c}})](x + z, x) . \end{aligned}$$



Therefore, for any  $(\hat{\mathbf{c}}, \hat{\mathbf{b}}) \in \mathcal{D}_{\uparrow, \downarrow}^{(2,1)}$ ,

$$\mathfrak{U}^* H^{(2,1)} \mathfrak{U}(\hat{\mathbf{c}}, \hat{\mathbf{b}}) = (\hat{\mathbf{c}}', \hat{\mathbf{b}}') \in \mathfrak{F}_{\uparrow, \downarrow}^{(2,1)},$$

where, for any  $k, k_{\uparrow\downarrow} \in [-\pi, \pi)^2$ ,

$$\begin{aligned} [\hat{\mathbf{c}}'(k)](k_{\uparrow\downarrow}) &= \epsilon (4 - \cos(k_{\uparrow\downarrow} - k) - \cos(k_{\uparrow\downarrow})) [\hat{\mathbf{c}}(k)](k_{\uparrow\downarrow}) \\ &\quad + U \int_{[-\pi, \pi)^2} [\hat{\mathbf{c}}(k)](k_{\uparrow\downarrow}) \mathbf{m}(d^2 k_{\uparrow\downarrow}) \\ &\quad + \hat{v}(k) (1 + 2e^{-\kappa} \cos(k_{\uparrow\downarrow} - k)) \hat{\mathbf{b}}(k), \\ \hat{\mathbf{b}}'(k) &= \epsilon h_b (2 - \cos(k)) \hat{\mathbf{b}}(k) \\ &\quad + \hat{v}(k) \int_{[-\pi, \pi)^2} (1 + 2e^{-\kappa} \cos(k_{\uparrow\downarrow} - k)) [\hat{\mathbf{c}}(k)](k_{\uparrow\downarrow}) \mathbf{m}(d^2 k_{\uparrow\downarrow}). \end{aligned}$$

By (41)–(47), it follows that  $\mathfrak{U}^* H^{(2,1)} \mathfrak{U} = A$  on the dense subspace  $\mathcal{D}_{\uparrow, \downarrow}^{(2,1)}$ . By the boundedness of both operators on  $\mathfrak{F}_{\uparrow, \downarrow}^{(2,1)}$ , we arrive at the first assertion. To prove that

$$\|A\|_{\text{op}} = \max_{k \in [-\pi, \pi)^2} \|A(k)\|_{\text{op}},$$

and thus the second assertion, note that

$$\|A\|_{\text{op}} = \text{ess sup}_{k \in [-\pi, \pi)^2} \|A(k)\|_{\text{op}}.$$

See Section 6.1. Now, to complete the proof, use the continuity of the map  $k \mapsto A(k)$ .  $\square$

By using Lemma 7 and Proposition 25, we can extract spectral properties of  $H^{(2,1)}$ . In particular, the spectrum  $\sigma(H^{(2,1)})$  of  $H^{(2,1)}$  is bounded from below by

$$E_0 := \inf \sigma(H^{(2,1)}) \geq \inf_{k \in [-\pi, \pi)^2} \{\min \sigma(A(k))\}. \quad (48)$$

In fact, the latter bound holds with equality:

**Lemma 8 (Bottom of the spectrum of  $H^{(2,1)}$ )**

*For any  $k \in [-\pi, \pi)^2$ , let  $\sigma_d(A(k))$  be the discrete spectrum of  $A(k)$ . Then*

$$\begin{aligned} E_0 &= \min \sigma(H^{(2,1)}) = \min_{k \in [-\pi, \pi)^2} \{\min \sigma(A(k))\} \\ &= \min \left\{ 0, \min_{k \in [-\pi, \pi)^2} \{\min \sigma_d(A(k))\} \right\} \leq 0. \end{aligned}$$

*Proof.* The operators  $A_{2,1}$ ,  $A_{1,2}$  and  $P_0$  are compact operators. Hence, for any  $k \in [-\pi, \pi]^2$ , the essential spectrum  $\sigma_{\text{ess}}(A(k))$  of  $A(k)$  equals

$$\sigma_{\text{ess}}(A(k)) = 2\epsilon \cos(k/2) \cdot [-1, 1] + 4\epsilon \subset [0, 8\epsilon] \quad (49)$$

for any  $\epsilon > 0$ , while  $\sigma_{\text{ess}}(A(k)) = \emptyset$  when  $\epsilon = 0$ . It follows from (48)–(49) and Proposition 25 together with Kato's theory for the perturbation of the discrete spectrum  $\sigma_d$  of closed operators that

$$E_0 = \min \sigma(H^{(2,1)}) = \min_{k \in [-\pi, \pi]^2} \{ \min \{ \sigma_{\text{ess}}(A(k)) \cup \sigma_d(A(k)) \} \} . \quad (50)$$

Since

$$\min_{k \in [-\pi, \pi]^2} \{ \min \sigma_{\text{ess}}(A(k)) \} = 0 , \quad (51)$$

we thus infer the assertion from (50).  $\square$

## 5.2 Negative Eigenvalues of the Fiber Hamiltonians

We analyze now the bottom of the spectrum of the fiber Hamiltonians  $A(k)$  for quasi-momenta  $k \in [-\pi, \pi]^2$ :

### Lemma 9 (Negative eigenvalues of $A(k) - \mathbf{I}$ )

Let  $k \in [-\pi, \pi]^2$  and  $\lambda < 0$ . Then,  $\lambda \in \sigma(A(k))$  if and only if  $v(k) \neq 0$  and there is  $\Psi_{\uparrow\downarrow} \in L^2([- \pi, \pi]^2, \mathfrak{m}; \mathbb{C}) \setminus \{0\}$  such that

$$[(A_{1,1}(k) - \lambda) - A_{1,2}(k)(A_{2,2}(k) - \lambda)^{-1}A_{2,1}(k)] \Psi_{\uparrow\downarrow} = 0 .$$

In this case,  $\lambda < 0$  is an eigenvalue of  $A(k)$  with associated eigenvector

$$(\Psi_{\uparrow\downarrow}, -(A_{2,2}(k) - \lambda)^{-1}A_{2,1}(k)\Psi_{\uparrow\downarrow}) \in L^2([- \pi, \pi]^2, \mathfrak{m}; \mathbb{C}) \setminus \{0\} \times \mathbb{C} \setminus \{0\} .$$

*Proof.* Fix  $k \in [-\pi, \pi]^2$  and  $\lambda < 0$ . Assume that  $\lambda \in \sigma(A(k))$ . Then  $\lambda \in \sigma_d(A(k))$ , by (49). For such a discrete eigenvalue there is  $\Psi_{\uparrow\downarrow} \in L^2([- \pi, \pi]^2, \mathfrak{m}; \mathbb{C})$  and  $\Psi_b \in \mathbb{C}$  such that  $(\Psi_{\uparrow\downarrow}, \Psi_b) \neq (0, 0)$  and

$$\begin{pmatrix} (A_{1,1}(k) - \lambda)\Psi_{\uparrow\downarrow} + A_{1,2}(k)\Psi_b \\ A_{2,1}(k)\Psi_{\uparrow\downarrow} + (A_{2,2}(k) - \lambda)\Psi_b \end{pmatrix} = \begin{pmatrix} 0 \\ 0 \end{pmatrix} , \quad (52)$$

see (46). From (41)–(42) and (45) with  $U, \epsilon, h_b \geq 0$  and  $\lambda < 0$ , note that  $A_{2,2}(k) - \lambda > 0$  and  $A_{1,1}(k) - \lambda > 0$ . This yields  $\Psi_{\uparrow\downarrow} \neq 0$ ,  $\Psi_b \neq 0$  and  $v(k) \neq 0$ .

Hence, if  $\lambda < 0$  then  $\lambda \in \sigma(A(k))$  if and only if (52) holds true with  $\Psi_{\uparrow\downarrow} \in L^2([-\pi, \pi]^2, \mathfrak{m}; \mathbb{C}) \setminus \{0\}$  and  $\Psi_b \in \mathbb{C} \setminus \{0\}$ . By combining the two equations of (52) we arrive at the assertion.  $\square$

We next analyze conditions for the existence of negative eigenvalues of  $A(k)$  for  $k \in [-\pi, \pi]^2$ . With this aim, we use the Birman–Schwinger principle (Proposition 26) to transform the eigenvalue problem (52) into a non–linear equation for  $\lambda$  on negative reals. This permits us to study afterwards the behavior of negative eigenvalues of  $A(k)$  as functions of the couplings  $\hat{v}$  and  $U$ .

**Proposition 10 (Negative eigenvalues of  $A(k)$  – II)**

*Let  $k \in [-\pi, \pi]^2$  and  $\lambda < 0$ . Then,  $\lambda \in \sigma(A(k))$  if and only if*

$$|\hat{v}(k)|^2 \mathcal{R}(k, U, \lambda) + \lambda - \epsilon h_b(2 - \cos(k)) = 0, \quad (53)$$

where

$$\mathcal{R}(k, U, \lambda) := \langle \mathfrak{d}(k) + \mathfrak{s}, (A_{1,1}(k) - \lambda)^{-1}(\mathfrak{d}(k) + \mathfrak{s}) \rangle. \quad (54)$$

*In this case,  $\lambda$  is a non–degenerated discrete eigenvalue of  $A(k)$ .*

*Proof.* Fix  $k \in [-\pi, \pi]^2$ . Since

$$\|\mathfrak{d}(k) + \mathfrak{s}\|_2^2 = \|\mathfrak{d}(k)\|_2^2 + \|\mathfrak{s}\|_2^2 = 4e^{-2\kappa} + 1, \quad (55)$$

note from (43)–(44) that

$$A_{1,2}(k)A_{2,1}(k) = (1 + 4e^{-2\kappa}) |\hat{v}(k)|^2 P_{\mathfrak{d}(k)},$$

where  $P_{\mathfrak{d}(k)}$  is the orthogonal projection with range (39). Because  $U, \epsilon, h_b \geq 0$ , recall that  $A_{1,1}(k) \geq 0$  and  $A_{2,2}(k) \geq 0$ , see (41)–(42) and (45). Hence, by applying Lemma 9 and Proposition 26 (Birman–Schwinger principle) to

$$H_0 = A_{1,1}(k) \quad \text{and} \quad V = A_{1,2}(k)(A_{2,2}(k) - \lambda)^{-1}A_{2,1}(k),$$

$\lambda < 0$  is an eigenvalue of  $A(k)$  if and only if

$$(1 + 4e^{-2\kappa}) |\hat{v}(k)|^2 P_{\mathfrak{d}(k)}(A_{1,1}(k) - \lambda)^{-1}P_{\mathfrak{d}(k)} = (\epsilon h_b(2 - \cos(k)) - \lambda)P_{\mathfrak{d}(k)}. \quad (56)$$

Note that  $P_{\mathfrak{d}(k)}$  is a rank one projector and hence, again by Proposition 26,  $\lambda$  is a non–degenerated eigenvalue of  $A(k)$ . So, we deduce the assertion from (55), (56) and the fact that  $\lambda \in \sigma(A(k))$  with  $\lambda < 0$  implies  $\lambda \in \sigma_d(A(k))$ , by (49).  $\square$

We next study the behavior of the function  $\mathcal{R}(k, U, \lambda)$  for negative spectral parameters  $\lambda < 0$  at any  $k \in [-\pi, \pi]^2$ .

**Lemma 11 (Behavior of the function  $\lambda \mapsto \mathcal{R}(k, U, \lambda)$ )**

Let  $k \in [-\pi, \pi)^2$  and  $U \geq 0$ . Then

$$\mathcal{R}(k, U, \lambda) = 4|\lambda|^{-1} e^{-2\kappa} + (U + |\lambda|)^{-1} + \mathcal{S}(k, U, \lambda)$$

is a strictly increasing function of  $\lambda < 0$  with

$$|\mathcal{S}(k, U, \lambda)| \leq 8\epsilon\lambda^{-2}(1 + 4e^{-2\kappa}) .$$

*Proof.* Fix in all the proof  $k \in [-\pi, \pi)^2$ ,  $U \geq 0$  and  $\lambda < 0$ . First, it is easy to check that the function  $\lambda \mapsto \mathcal{R}(k, U, \lambda)$  is strictly increasing for negative  $\lambda < 0$ , by strict positivity of the operator  $(A_{1,1}(k) - \lambda)^{-2}$  when  $\epsilon, U \geq 0$ . Secondly, by using (41)–(42) and the second resolvent equation we obtain

$$(A_{1,1}(k) - \lambda)^{-1} = (UP_0 - \lambda)^{-1} - (UP_0 - \lambda)^{-1}A_{1,1}^{(0)}(k)(A_{1,1}(k) - \lambda)^{-1} . \quad (57)$$

Clearly,

$$\|(UP_0 - \lambda)^{-1}\|_{\text{op}}, \|(A_{1,1}(k) - \lambda)^{-1}\|_{\text{op}} \leq |\lambda|^{-1} \quad \text{and} \quad \|A_{1,1}^{(0)}(k)\|_{\text{op}} \leq 8\epsilon .$$

It follows that

$$\|(A_{1,1}(k) - \lambda)^{-1} - (UP_0 - \lambda)^{-1}\|_{\text{op}} \leq 8\epsilon\lambda^{-2} .$$

Therefore, from (54) and (55),

$$|\mathcal{R}(k, U, \lambda) - \langle \mathfrak{d}(k) + \mathfrak{s}, (UP_0 - \lambda)^{-1}(\mathfrak{d}(k) + \mathfrak{s}) \rangle| \leq 8\epsilon\lambda^{-2}(1 + 4e^{-2\kappa}) . \quad (58)$$

Meanwhile, recall that  $P_0$  is the orthogonal projection with range (40) while  $\langle \mathfrak{d}(k), \mathfrak{s} \rangle = 0$ . Therefore,

$$\begin{aligned} & \langle \mathfrak{d}(k) + \mathfrak{s}, (UP_0 - \lambda)^{-1}(\mathfrak{d}(k) + \mathfrak{s}) \rangle \\ &= \langle \mathfrak{d}(k), (UP_0 - \lambda)^{-1}\mathfrak{d}(k) \rangle + \langle \mathfrak{s}, (UP_0 - \lambda)^{-1}\mathfrak{s} \rangle \\ &= |\lambda|^{-1} \langle \mathfrak{d}(k), \mathfrak{d}(k) \rangle + (U + |\lambda|)^{-1} \langle \mathfrak{s}, \mathfrak{s} \rangle , \end{aligned}$$

which, combined with (58), yields the assertion.  $\square$

From Proposition 10 and Lemma 11 we deduce the possible existence of a unique negative eigenvalue:

**Theorem 12 (Estimates on the negative eigenvalue of  $A(k)$ )**

Let  $k \in [-\pi, \pi)^2$ ,  $h_b \in [0, 1]$ ,  $U \geq 0$  and set

$$\epsilon_0 := \frac{e^{-2\kappa}}{4(1 + 4e^{-2\kappa})} e^{-\kappa}, \quad \kappa > 0.$$

(i) *There is at most one negative eigenvalue  $E(k) < 0$  of  $A(k)$ . If it exists,  $E(k)$  is non-degenerated.*

(ii) *If  $0 \leq \epsilon \leq \epsilon_0 |\hat{v}(k)|$  with  $|\hat{v}(k)| \neq 0$  then there is a negative eigenvalue  $E(k) \equiv E(k, U, \epsilon)$  of  $A(k)$  that satisfies*

$$e^{-\kappa} |\hat{v}(k)| < |E(k)| < |\hat{v}(k)| \sqrt{1 + 5e^{-2\kappa}}.$$

*Proof.* (i) Use Proposition 10 and the monotonicity of the map  $\lambda \mapsto \mathcal{R}(k, U, \lambda)$  on  $\mathbb{R}^-$  (Lemma 11).

(ii) Fix  $k \in [-\pi, \pi)^2$ ,  $h_b \in [0, 1]$  and  $U \geq 0$ . Assume that  $|\hat{v}(k)| \neq 0$ , let  $x := e^{-\kappa} |\hat{v}(k)|$  and take  $\epsilon \geq 0$  such that

$$0 \leq \epsilon \leq \epsilon_0 |\hat{v}(k)| < \frac{x}{4}. \quad (59)$$

Then, by Lemma 11,

$$\begin{aligned} & |\hat{v}(k)|^2 \mathcal{R}(k, U, -x) - 2x \\ &= |\hat{v}(k)|^2 (4x^{-1}e^{-2\kappa} + (U+x)^{-1} + \mathcal{S}(k, U, -x)) - 2x \\ &\geq |\hat{v}(k)|^2 4(x^{-1}e^{-2\kappa} - 2\epsilon x^{-2}(1 + 4e^{-2\kappa})) - 2x \\ &\geq |\hat{v}(k)|^2 2x^{-1}e^{-2\kappa} - 2x = 0. \end{aligned}$$

Recall now that  $\mathcal{R}(k, U, \lambda) > 0$  is a strictly positive and increasing function of  $\lambda < 0$ , by Lemma 11. Therefore, for any parameter  $\epsilon$  satisfying (59), there is a solution  $E(k)$  of (53) that satisfies  $|E(k)| > x$ . Note that one also uses here  $h_b \in [0, 1]$ .

Now, take

$$y = |\hat{v}(k)| \sqrt{1 + 5e^{-2\kappa}},$$

where we recall that  $|\hat{v}(k)| \neq 0$ . Then, using (59) and Lemma 11, we obtain that

$$\begin{aligned} |\hat{v}(k)|^2 \mathcal{R}(k, U, -y) - y &\leq |\hat{v}(k)|^2 y^{-1} (4e^{-2\kappa} + 1 + 8\epsilon y^{-1}(1 + 4e^{-2\kappa})) - y \\ &\leq \frac{|\hat{v}(k)| e^{-3\kappa}}{(1 + 5e^{-2\kappa})} \left( 2 - \sqrt{5 + e^{2\kappa}} \right) < 0. \end{aligned}$$

Then, by Lemma 11, if  $\epsilon$  satisfies (59), there is a solution  $E(k)$  of (53) satisfying  $|E(k)| < y$ .  $\square$

We now conclude this subsection by proving the existence of a bound fermion pair whenever the bottom  $E_0$  of the spectrum of  $H^{(2,1)}$  is strictly negative:

**Proposition 13 (Bound fermion pair formation at strictly negative energy – I)**  
Assume that  $E_0 < 0$  and take any  $(\mathbf{c}_0, \mathbf{b}_0) \in \mathfrak{H}_\varepsilon \setminus \{0\}$  with  $\varepsilon \in (0, 1)$ . Let

$$(\mathbf{c}_t, \mathbf{b}_t) := e^{-itH^{(2,1)}}(\mathbf{c}_0, \mathbf{b}_0), \quad t \in \mathbb{R}.$$

(i) *Non-vanishing fermion component:*

$$\|\mathbf{c}_t\|_2 = \|\mathbf{c}_0\|_2 > 0, \quad t \in \mathbb{R}.$$

(ii) *Bound fermion pair formation:*

$$\lim_{R \rightarrow \infty} \sum_{x_\uparrow, x_\downarrow \in \mathbb{Z}^2: |x_\uparrow - x_\downarrow| \leq R} |\mathbf{c}_t(x_\uparrow, x_\downarrow)|^2 = \|\mathbf{c}_0\|_2^2,$$

uniformly with respect to  $t \in \mathbb{R}$ .

*Proof.* (i) For any  $t \in \mathbb{R}$ , let  $(\hat{\mathbf{c}}_t, \hat{\mathbf{b}}_t) := \mathfrak{U}^*(\mathbf{c}_t, \mathbf{b}_t)$ , see (37). If  $E_0 < 0$  and  $(\mathbf{c}_0, \mathbf{b}_0) \in \mathfrak{H}_\varepsilon$ , then we infer from Lemma 8, Equation (49) and Theorem 12 (i) together with Proposition 25 (iii) that

$$(\mathbf{c}_t, \mathbf{b}_t) = \mathfrak{U} \left( \int_{[-\pi, \pi]^2}^{\oplus} e^{-itE(k)} (\hat{\mathbf{c}}_0(k), \hat{\mathbf{b}}_0(k)) \, \mathbf{m}(d^2k) \right) \quad (60)$$

for any  $t \in \mathbb{R}$ , where, by Lemma 9,

$$\hat{\mathbf{c}}_0(k) = 0 \quad \text{if and only if} \quad \hat{\mathbf{b}}_0(k) = 0. \quad (61)$$

This implies Assertion (i), because

$$\|\mathbf{c}_t\|_2^2 = \int_{[-\pi, \pi]^2} \|\hat{\mathbf{c}}_0(k)\|_2^2 \, \mathbf{m}(d^2k) = \|\mathbf{c}_0\|_2^2. \quad (62)$$

(ii) By (60), there is a family  $\{P^{(R)}\}_{R \in \mathbb{R}^+}$  of orthogonal projectors acting on  $L^2([-\pi, \pi]^2, \mathbf{m}; \mathbb{C})$ , converging strongly to the identity as  $R \rightarrow \infty$ , and such that

$$\sum_{x_\uparrow, x_\downarrow \in \mathbb{Z}^2: |x_\uparrow - x_\downarrow| \leq R} |\mathbf{c}_t(x_\uparrow, x_\downarrow)|^2 = \int_{[-\pi, \pi]^2} \|P^{(R)} \hat{\mathbf{c}}_0(k)\|_2^2 \, \mathbf{m}(d^2k). \quad (63)$$

By Lebesgue's dominated convergence theorem, Assertion (ii) then follows.  $\square$

### 5.3 Coefficients $\mathcal{R}(k, U, \lambda)$ in terms of Explicit Integrals

To prove Theorem 2, we need to express the positive numbers  $\mathcal{R}(k, U, \lambda)$  for  $k \in [-\pi, \pi]^2$ ,  $U \geq 0$  and  $\lambda < 0$  in terms of the explicit quantities  $R_{\mathfrak{s}, \mathfrak{s}}^{(0)}$ ,  $R_{\mathfrak{d}, \mathfrak{d}}^{(0)}$ , and  $R_{\mathfrak{s}, \mathfrak{d}}^{(0)}$  defined by (16)–(18). See Proposition 10 for the definition and the use of  $\mathcal{R}(k, U, \lambda)$ . This is done in the following lemma:

**Lemma 14 (Explicit expression for  $\mathcal{R}(k, U, \lambda)$ )**

Let  $k \in [-\pi, \pi]^2$ ,  $U \geq 0$  and  $\lambda < 0$ . Then

$$\mathcal{R}(k, U, \lambda) = \frac{R_{\mathfrak{d}, \mathfrak{d}}^{(0)}}{1 + UR_{\mathfrak{s}, \mathfrak{s}}^{(0)}} + U \frac{R_{\mathfrak{d}, \mathfrak{d}}^{(0)} R_{\mathfrak{s}, \mathfrak{s}}^{(0)} - (R_{\mathfrak{s}, \mathfrak{d}}^{(0)})^2}{1 + UR_{\mathfrak{s}, \mathfrak{s}}^{(0)}}$$

with

$$\frac{R_{\mathfrak{d}, \mathfrak{d}}^{(0)}}{1 + UR_{\mathfrak{s}, \mathfrak{s}}^{(0)}} > 0 \quad \text{and} \quad U \frac{R_{\mathfrak{d}, \mathfrak{d}}^{(0)} R_{\mathfrak{s}, \mathfrak{s}}^{(0)} - (R_{\mathfrak{s}, \mathfrak{d}}^{(0)})^2}{1 + UR_{\mathfrak{s}, \mathfrak{s}}^{(0)}} \geq 0. \quad (64)$$

*Proof.* Fix  $k \in [-\pi, \pi]^2$ ,  $U \geq 0$  and  $\lambda < 0$ . From Definitions (16)–(18), (38), and (41), note that

$$\begin{aligned} R_{\mathfrak{s}, \mathfrak{s}}^{(0)} &= \left\langle \mathfrak{s}, (A_{1,1}^{(0)}(k) - \lambda)^{-1} \mathfrak{s} \right\rangle, \\ R_{\mathfrak{d}, \mathfrak{d}}^{(0)} &= \left\langle \mathfrak{d}(k) + \mathfrak{s}, (A_{1,1}^{(0)}(k) - \lambda)^{-1} (\mathfrak{d}(k) + \mathfrak{s}) \right\rangle, \\ R_{\mathfrak{s}, \mathfrak{d}}^{(0)} &= \left\langle \mathfrak{s}, (A_{1,1}^{(0)}(k) - \lambda)^{-1} (\mathfrak{d}(k) + \mathfrak{s}) \right\rangle. \end{aligned}$$

Define the real numbers

$$\begin{aligned} R_{\mathfrak{s}, \mathfrak{s}} &:= \left\langle \mathfrak{s}, (A_{1,1}(k) - \lambda)^{-1} \mathfrak{s} \right\rangle, \\ R_{\mathfrak{d}, \mathfrak{d}} &:= \left\langle \mathfrak{d}(k) + \mathfrak{s}, (A_{1,1}(k) - \lambda)^{-1} (\mathfrak{d}(k) + \mathfrak{s}) \right\rangle, \\ R_{\mathfrak{s}, \mathfrak{d}} &:= \left\langle \mathfrak{s}, (A_{1,1}(k) - \lambda)^{-1} (\mathfrak{d}(k) + \mathfrak{s}) \right\rangle. \end{aligned} \quad (65)$$

and observe that  $R_{\mathfrak{d}, \mathfrak{d}}$  is only another notation for  $\mathcal{R}(k, U, \lambda)$ :

$$R_{\mathfrak{d}, \mathfrak{d}} = \mathcal{R}(k, U, \lambda). \quad (66)$$

From the resolvent equation

$$(A_{1,1}(k) - \lambda)^{-1} = (A_{1,1}^{(0)}(k) - \lambda)^{-1} - U(A_{1,1}^{(0)}(k) - \lambda)^{-1} P_0 (A_{1,1}(k) - \lambda)^{-1} \quad (67)$$

(see (42)), we arrive at the linear system

$$\begin{pmatrix} R_{s,s} & R_{s,d} \\ R_{s,d} & R_{d,d} \end{pmatrix} = -U \begin{pmatrix} R_{s,s}^{(0)} R_{s,s} & R_{s,s}^{(0)} R_{s,d} \\ R_{s,d}^{(0)} R_{s,s} & R_{s,d}^{(0)} R_{d,d} \end{pmatrix} + \begin{pmatrix} R_{s,s}^{(0)} & R_{s,d}^{(0)} \\ R_{s,d}^{(0)} & R_{d,d}^{(0)} \end{pmatrix} \\ = - \begin{pmatrix} UR_{s,s}^{(0)} & 0 \\ UR_{s,d}^{(0)} & 0 \end{pmatrix} \begin{pmatrix} R_{s,s} & R_{s,d} \\ R_{s,d} & R_{d,d} \end{pmatrix} + \begin{pmatrix} R_{s,s}^{(0)} & R_{s,d}^{(0)} \\ R_{s,d}^{(0)} & R_{d,d}^{(0)} \end{pmatrix},$$

which means

$$\begin{pmatrix} UR_{s,s}^{(0)} + 1 & 0 \\ UR_{s,d}^{(0)} & 1 \end{pmatrix} \begin{pmatrix} R_{s,s} & R_{s,d} \\ R_{s,d} & R_{d,d} \end{pmatrix} = \begin{pmatrix} R_{s,s}^{(0)} & R_{s,d}^{(0)} \\ R_{s,d}^{(0)} & R_{d,d}^{(0)} \end{pmatrix}.$$

Note that, by positivity of the constants  $R_{s,s}^{(0)} \geq 0$  and  $U \geq 0$ , the matrix

$$\begin{pmatrix} UR_{s,s}^{(0)} + 1 & 0 \\ UR_{s,d}^{(0)} & 1 \end{pmatrix}$$

is invertible and we obtain

$$\begin{pmatrix} R_{s,s} & R_{s,d} \\ R_{s,d} & R_{d,d} \end{pmatrix} = \frac{1}{1 + UR_{s,s}^{(0)}} \begin{pmatrix} 1 & 0 \\ -UR_{s,d}^{(0)} & UR_{s,s}^{(0)} + 1 \end{pmatrix} \begin{pmatrix} R_{s,s}^{(0)} & R_{s,d}^{(0)} \\ R_{s,d}^{(0)} & R_{d,d}^{(0)} \end{pmatrix}.$$

In particular,

$$R_{d,d} = \frac{R_{d,d}^{(0)}(1 + UR_{s,s}^{(0)}) - U(R_{s,d}^{(0)})^2}{1 + UR_{s,s}^{(0)}} = \frac{R_{d,d}^{(0)}}{1 + UR_{s,s}^{(0)}} + U \frac{R_{d,d}^{(0)}R_{s,s}^{(0)} - (R_{s,d}^{(0)})^2}{1 + UR_{s,s}^{(0)}},$$

which, combined with (66), implies the assertion. Note that the second inequality of (64) follows from the positivity of the operator  $(A_{1,1}^{(0)}(k) - \lambda)^{-1}$ .  $\square$

The behavior of  $\mathcal{R}(k, U, \lambda)$  at large Hubbard coupling  $U \geq 0$  can now be deduced. This is useful for the proof of Theorem 2 (ii).

**Lemma 15** ( $\mathcal{R}(k, U, \lambda)$  at large  $U \geq 0$ )

For any  $k \in [-\pi, \pi)^2$ ,  $U \geq 0$  and  $\lambda < 0$ .

$$4e^{-2\kappa} (|\lambda| + 4\epsilon)^{-1} + (U + 4\epsilon + |\lambda|)^{-1} \leq \mathcal{R}(k, U, \lambda) \leq 4e^{-2\kappa} |\lambda|^{-1} + (U + |\lambda|)^{-1} \quad (68)$$

and for any  $U > 0$ ,

$$\left| \mathcal{R}(k, U, \lambda) - \frac{R_{d,d}^{(0)}R_{s,s}^{(0)} - (R_{s,d}^{(0)})^2}{R_{s,s}^{(0)}} \right| < (1 + 4e^{-\kappa})^2 U^{-1}. \quad (69)$$



*Proof.* The Inequalities (68) are direct consequences of the definition of  $\mathcal{R}(k, U, \lambda)$  (see, e.g., (65) and (66)) and the fact that  $A^{-1} \leq B^{-1}$  for any strictly positive operators  $A, B > 0$  with  $B \leq A$ . Moreover, we infer from Lemma 14 that

$$\mathcal{R}(k, U, \lambda) - \frac{R_{\mathfrak{s},\mathfrak{s}}^{(0)} R_{\mathfrak{s},\mathfrak{s}}^{(0)} - (R_{\mathfrak{s},\mathfrak{s}}^{(0)})^2}{R_{\mathfrak{s},\mathfrak{s}}^{(0)}} = \frac{(R_{\mathfrak{s},\mathfrak{s}}^{(0)})^2}{(1 + U R_{\mathfrak{s},\mathfrak{s}}^{(0)}) R_{\mathfrak{s},\mathfrak{s}}^{(0)}}. \quad (70)$$

Note that  $R_{\mathfrak{s},\mathfrak{s}}^{(0)} > 0$ , by strict positivity of  $(A_{1,1}^{(0)}(k) - \lambda)^{-1} > 0$ . Since, by (16) and (18),

$$|R_{\mathfrak{s},\mathfrak{s}}^{(0)}| \leq (1 + 4e^{-\kappa}) R_{\mathfrak{s},\mathfrak{s}}^{(0)},$$

we thus deduce from (70) Inequality (69) for any  $U > 0$ .  $\square$

## 5.4 Pairing Mode of Fermions with Minimum Energy

Recall that if at quasi-momentum  $k \in [-\pi, \pi)^2$ ,

$$0 \leq \epsilon \leq \epsilon_0 |\hat{v}(k)| = \frac{e^{-2\kappa}}{4(1 + 4e^{-2\kappa})} e^{-\kappa} |\hat{v}(k)|,$$

then there is a unique negative eigenvalue  $E(k) \equiv E(k, U, \epsilon)$  of  $A(k)$  for any  $h_b \in [0, 1]$  and  $U \geq 0$ . See Theorem 12. In this section, we are interested in the asymptotics of  $E(k)$  in the limits of small kinetic terms  $\epsilon \rightarrow 0^+$  and large or small Hubbard repulsions  $U \rightarrow \infty, 0^+$ . We start by general results which hold for any  $U \geq 0$ , provided  $\epsilon \leq \tilde{\epsilon}_0 |\hat{v}(k)|$  with

$$\tilde{\epsilon}_0 := \frac{e^{-2\kappa}}{4} \min \left\{ \frac{1}{6\sqrt{1 + 5e^{-2\kappa}}}, \frac{e^{-\kappa}}{(1 + 4e^{-2\kappa})} \right\} \leq \epsilon_0. \quad (71)$$

### Theorem 16 (Asymptotics of the negative eigenvalue of $A(k) - \mathbf{I}$ )

There is a constant  $D_\kappa < \infty$  depending only on  $\kappa > 0$  such that, for every  $h_b \in [0, 1]$ ,  $U \geq 0$ ,  $k \in [-\pi, \pi)^2$  and any parameter  $\epsilon \geq 0$  satisfying  $0 \leq \epsilon < \tilde{\epsilon}_0 |\hat{v}(k)|$ , one has:

(i) *Negative (non-degenerated) eigenvalue of  $A(k)$ :*

$$\left| E(k) + \frac{|\hat{v}(k)|}{2} \left( \frac{|\hat{v}(k)|}{U - E(k)} + \sqrt{16e^{-2\kappa} + \frac{|\hat{v}(k)|^2}{(U - E(k))^2}} \right) \right| \leq \epsilon D_\kappa.$$

(ii) *Eigenvector: There is an eigenvector*

$$(\Psi_{\uparrow\downarrow}(k), \Psi_b(k)) \equiv (\Psi_{\uparrow\downarrow}(k, U, \hat{v}), \Psi_b(k, U, \hat{v}))$$

associated with  $E(k)$  such that

$$\left\| \Psi_{\uparrow\downarrow}(k) - \left( \frac{e^{2\kappa}}{4} \left( \frac{E(k)}{\hat{v}(k)} + \frac{\hat{v}(k)}{U - E(k)} \right) \mathfrak{d}(k) - \frac{\hat{v}(k)}{U - E(k)} \mathfrak{s} \right) \right\|_2 \leq \epsilon |\hat{v}(k)|^{-1} D_\kappa$$

and

$$|\Psi_b(k) - 1| \leq \epsilon |\hat{v}(k)|^{-1} D_\kappa. \quad (72)$$

*Proof.* Similarly to  $A(k)$ , for any  $U \geq 0$  and  $k \in [-\pi, \pi)^2$ , let

$$B(k) := \begin{pmatrix} UP_0 & A_{1,2}(k) \\ A_{2,1}(k) & 0 \end{pmatrix} \in \mathcal{B}(L^2([-\pi, \pi)^2, \mathfrak{m}; \mathbb{C}) \times \mathbb{C}),$$

where  $P_0$  is the orthogonal projection with range (40). Compare this with (41)–(46) in the limit  $\epsilon \rightarrow 0^+$  to see that  $B(k) = A(k)|_{\epsilon=0}$ . Therefore, by Theorem 12, if  $\hat{v}(k) \neq 0$  then there is a negative eigenvalue  $F(k)$  of  $B(k)$  that satisfies

$$e^{-\kappa} |\hat{v}(k)| < |F(k)| < |\hat{v}(k)| \sqrt{1 + 5e^{-2\kappa}}. \quad (73)$$

This eigenvalue is moreover non-degenerated and the unique strictly negative eigenvalue of  $B(k)$ . In fact, it can be explicitly computed together with its eigenvector.

Indeed, for any  $k \in [-\pi, \pi)^2$ , let

$$\Phi_{\uparrow\downarrow}(k) := \frac{e^{2\kappa}}{4} \left( \frac{F(k)}{\hat{v}(k)} + \frac{\hat{v}(k)}{U - F(k)} \right) \mathfrak{d}(k) - \frac{\hat{v}(k)}{U - F(k)} \mathfrak{s}. \quad (74)$$

Then, by explicit computations, observe that  $(\Phi_{\uparrow\downarrow}(k), 1)$  is an eigenvector of  $B(k)$  associated with the eigenvalue

$$F(k) = -\frac{|\hat{v}(k)|}{2} \left( \frac{|\hat{v}(k)|}{U - F(k)} + \sqrt{16e^{-2\kappa} + \left( \frac{|\hat{v}(k)|}{U - F(k)} \right)^2} \right) < 0. \quad (75)$$

Observe that a solution  $F(k) < 0$  of (75) always exists. Indeed,  $F(k) < 0$  solves (75) if and only if  $\xi(F(k)) = 4e^{-2\kappa}$ , where

$$\xi(x) := \frac{x^2}{|\hat{v}(k)|^2} + \frac{x}{U - x}, \quad x < 0. \quad (76)$$

Note that  $\xi(x) \rightarrow \infty$ , as  $x \rightarrow -\infty$ , and

$$x_0 = \frac{1}{2} \left( U - \sqrt{U^2 + 4|\hat{v}(k)|^2} \right)$$

is the unique strictly negative solution of  $\xi(x) = 0$ . Therefore, by continuity of  $\xi$  on  $-\mathbb{R}_0^+$ , there is a solution  $x_1 < x_0$  of (76). Hence (75) holds for some  $F(k) < 0$ .

By Theorem 12 (ii), if  $\epsilon \leq \epsilon_0 |\hat{v}(k)|$  with  $\hat{v}(k) \neq 0$  then there is a strictly negative and non degenerated eigenvalue  $E(k)$  of  $A(k)$ . This eigenvalue is close to  $F(k)$  for  $\epsilon \ll 1$  because of the equality  $B(k) = A(k)|_{\epsilon=0}$  and Kato's perturbation theory.

Indeed, let

$$\mathfrak{z}(k) := \frac{1}{2} \left( \sqrt{1 + 5e^{-2\kappa}} + e^{-\kappa} \right), \quad k \in [-\pi, \pi)^2, \quad (77)$$

and  $\mathcal{C}$  be the contour defined by

$$\mathcal{C}(y) := |\hat{v}(k)| \left( -\mathfrak{z}(k) + \left( \mathfrak{z}(k) - \frac{e^{-\kappa}}{2} \right) e^{2\pi i y} \right) \in \mathbb{C}, \quad y \in [0, 1], \quad (78)$$

for any  $k \in [-\pi, \pi)^2$  with  $\hat{v}(k) \neq 0$ . Then, we define the Riesz projections associated with  $E(k)$  and  $F(k)$  respectively by

$$\mathbf{P}^{(E(k))} := \frac{1}{2\pi i} \oint_{\mathcal{C}} (\zeta - A(k))^{-1} d\zeta \quad \text{and} \quad \mathbf{P}^{(F(k))} := \frac{1}{2\pi i} \oint_{\mathcal{C}} (\zeta - B(k))^{-1} d\zeta.$$

Both operators are well-defined for any  $h_b \in [0, 1]$ ,  $U \geq 0$ ,  $k \in [-\pi, \pi)^2$  with  $\hat{v}(k) \neq 0$  and  $\epsilon \leq \epsilon_0 |\hat{v}(k)|$  because of Theorem 12, see also (73). Using the resolvent equation,

$$\mathbf{P}^{(E(k))} - \mathbf{P}^{(F(k))} = \frac{1}{2\pi i} \oint_{\mathcal{C}} (\zeta - B(k))^{-1} (A(k) - B(k)) (\zeta - A(k))^{-1} d\zeta$$

from which we deduce

$$\begin{aligned} \|\mathbf{P}^{(E(k))} - \mathbf{P}^{(F(k))}\|_{\text{op}} &\leq \frac{2e^{2\kappa} \sqrt{1 + 5e^{-2\kappa}}}{|\hat{v}(k)|} \left( \|A_{1,1}^{(0)}(k)\|_{\text{op}} + \|A_{2,2}(k)\|_{\text{op}} \right) \\ &\leq 24e^{2\kappa} \sqrt{1 + 5e^{-2\kappa}} |\hat{v}(k)|^{-1} \epsilon \end{aligned} \quad (79)$$

for any  $h_b \in [0, 1]$ ,  $U \geq 0$ ,  $k \in [-\pi, \pi)^2$  such that  $\hat{v}(k) \neq 0$ , and parameters  $\epsilon \leq \epsilon_0 |\hat{v}(k)|$ . See Theorem 12 and Equations (41)–(46), (49), (73) and (77)–(78). Since

$$\mathbf{P}^{(F(k))}(\Phi_{\uparrow\downarrow}(k), 1) = (\Phi_{\uparrow\downarrow}(k), 1) , \quad (80)$$

it follows that, for any  $h_b \in [0, 1]$ ,  $U \geq 0$ ,  $k \in [-\pi, \pi)^2$  such that  $\hat{v}(k) \neq 0$ , and parameters  $\epsilon < \tilde{\epsilon}_0 |\hat{v}(k)|$  (cf. (71)), the vector

$$(\Psi_{\uparrow\downarrow}(k), \Psi_b(k)) := \mathbf{P}^{(E(k))}(\Phi_{\uparrow\downarrow}(k), 1) \neq 0 \quad (81)$$

is an eigenvector of  $A(k)$  associated with the unique strictly negative eigenvalue  $E(k)$  of  $A(k)$  while

$$|E(k) - F(k)| \leq 12\epsilon . \quad (82)$$

By combining (79)–(82) with Theorem 12 (ii) and (74)–(75) we arrive at the assertions from direct estimates. Note only that  $D_\kappa$  is a function of  $e^{2\kappa}$  exponentially growing to infinity when  $\kappa \rightarrow \infty$ .  $\square$

Clearly,

$$\|\Psi_{\uparrow\downarrow}(k)\|_2^2 = 1 - |\Psi_b(k)|^2 \leq 1$$

is the probability of finding a pair of fermions, and not a boson, with quasi-momentum  $k \in [-\pi, \pi)^2$ . Similarly,  $|\Psi_b(k)|^2$  is the probability of finding a boson with the same quasi-momentum. The norm-one function  $\|\Psi_{\uparrow\downarrow}(k)\|_2^{-1} \Psi_{\uparrow\downarrow}(k)$  describes the orbital structure of the bound fermion pair. Theorem 16 says that, for small parameters  $\epsilon \leq \tilde{\epsilon}_0 |\hat{v}(k)|$ , the orbital structure of the bound fermion pair has mainly  $s$ - and  $d$ -wave components. This fact holds true even in the limit  $U \rightarrow 0^+$ :

### Corollary 17 (Asymptotics of the negative eigenvalue of $A(k)$ – II)

*There is a constant  $D_\kappa < \infty$  depending only on  $\kappa > 0$  such that, for every  $h_b \in [0, 1]$ ,  $U \geq 0$ ,  $k \in [-\pi, \pi)^2$  and any parameter  $\epsilon \geq 0$  satisfying  $0 \leq \epsilon < \tilde{\epsilon}_0 |\hat{v}(k)|$ , one has:*

(i) *Negative (non-degenerated) eigenvalue of  $A(k)$ :*

$$\left| E(k) + |\hat{v}(k)| \sqrt{1 + 4e^{-2\kappa}} \right| \leq D_\kappa (\epsilon + U) .$$

(ii) *Eigenvector: There is an eigenvector  $(\Psi_{\uparrow\downarrow}(k), \Psi_b(k))$  associated with  $E(k)$  such that (72) holds and*

$$\|\Psi_{\uparrow\downarrow}(k) + \mathfrak{d}(k) + \mathfrak{s}\|_2 \leq D_\kappa (\epsilon |\hat{v}(k)|^{-1} + U) .$$

In contrast to  $U \ll 1$ , in the limit of large Hubbard couplings  $U \gg 1$  the  $s$ -wave component of the orbital structure of the bound fermion pair is suppressed by the Hubbard repulsion without changing (at leading order) the binding energy of the particles.

**Corollary 18 (Asymptotics of the negative eigenvalue of  $A(k)$  – III)**

There is a constant  $D_\kappa < \infty$  depending only on  $\kappa > 0$  such that, for every  $h_b \in [0, 1]$ ,  $U \geq 0$ ,  $k \in [-\pi, \pi)^2$  and any parameter  $\epsilon \geq 0$  satisfying  $0 \leq \epsilon < \tilde{\epsilon}_0 |\hat{v}(k)|$ , one has:

(i) *Negative (non-degenerated) eigenvalue of  $A(k)$ :*

$$\left| E(k) + 2e^{-\kappa} |\hat{v}(k)| + \frac{|\hat{v}(k)|^2}{2U} \right| \leq D_\kappa (\epsilon + U^{-2}) .$$

(ii) *Eigenvector: There is an eigenvector  $(\Psi_{\uparrow\downarrow}(k), \Psi_b(k))$  associated with  $E(k)$  such that (72) holds and*

$$\left\| \Psi_{\uparrow\downarrow}(k) - \frac{e^\kappa}{2} \text{sgn}(\hat{v}(k)) \mathfrak{d}(k) - \frac{\hat{v}(k)}{U} \mathfrak{s} \right\|_2 \leq D_\kappa (\epsilon |\hat{v}(k)|^{-1} + U^{-2}) .$$

Note that Corollaries 17–18 and the operator monotonicity of  $A_{1,1}(k)$  with respect to  $U$  imply that, for all  $k \in [-\pi, \pi)^2$  with  $\epsilon < \tilde{\epsilon}_0 |\hat{v}(k)|$ , and every  $h_b \in [0, 1]$  and  $U \geq 0$ ,

$$2e^{-\kappa} |\hat{v}(k)| + \mathcal{O}(\epsilon) \leq |E(k)| \leq |\hat{v}(k)| \sqrt{1 + 4e^{-2\kappa}} + \mathcal{O}(\epsilon) .$$

Compare with Theorem 12 (ii).

By definition of  $\mathfrak{d}(k)$  (see (38)), observe that

$$\left\| \frac{e^\kappa}{2} \text{sgn}(\hat{v}(k)) \mathfrak{d}(k) \right\|_2 = 1$$

for all  $\kappa \in \mathbb{R}_0^+$ . Hence, the fact that orbital of the bound pair is of  $d$ -wave type only depends on  $|\hat{v}(k)| U^{-1}$  being small.

Recall that Proposition 13 shows the existence of a bound fermion pair whenever the bottom  $E_0$  of the spectrum of  $H^{(2,1)}$  is strictly negative. In this case, for any  $(\mathfrak{c}_0, \mathfrak{b}_0) \in \mathfrak{H}_\varepsilon \setminus \{0\}$  with  $\varepsilon \in (0, 1)$ ,

$$(\mathfrak{c}_t, \mathfrak{b}_t) := e^{-itH^{(2,1)}}(\mathfrak{c}_0, \mathfrak{b}_0) , \quad t \in \mathbb{R} , \quad (83)$$

has a non-vanishing fermion component, i.e.,  $\|\mathbf{c}_t\|_2 = \|\mathbf{c}_0\|_2 > 0$ . By explicit computations, one checks that the  $s$ - and  $d$ -wave components of the orbital structure of the bound fermion pair both corresponds in the lattice  $\mathbb{Z}^2$  to wave functions with a fermion pair localized in a ball of radius 1. Therefore, by using Theorem 16, we can improve Proposition 13 (ii):

**Corollary 19 (Bound fermion pair formation at strictly negative energy - II)**

Assume  $E_0 < 0$  and let  $(\mathbf{c}_t, \mathbf{b}_t)$  be defined by (83) for any  $t \in \mathbb{R}$  and  $(\mathbf{c}_0, \mathbf{b}_0) \in \mathfrak{H}_\varepsilon \setminus \{0\}$  with  $\varepsilon \in (0, 1)$ . Then, uniformly with respect to  $t \in \mathbb{R}$  and  $(\mathbf{c}_0, \mathbf{b}_0) \in \mathfrak{H}_\varepsilon \setminus \{0\}$ ,

$$\lim_{\varepsilon \rightarrow 0^+} \left\{ \|\mathbf{c}_0\|_2^{-2} \sum_{x_\uparrow, x_\downarrow \in \mathbb{Z}^2: |x_\uparrow - x_\downarrow| \leq 1} |\mathbf{c}_t(x_\uparrow, x_\downarrow)|^2 \right\} = 1 .$$

*Proof.* From (63),

$$\sum_{x_\uparrow, x_\downarrow \in \mathbb{Z}^2: |x_\uparrow - x_\downarrow| \leq 1} |\mathbf{c}_t(x_\uparrow, x_\downarrow)|^2 = \int_{[-\pi, \pi]^2} \|P^{(1)} \hat{\mathbf{c}}_0(k)\|_2^2 \, \mathbf{m}(d^2 k) . \quad (84)$$

Theorems 12 (ii) and 16 (ii) imply the existence of  $D < \infty$  such that, for all  $k \in [-\pi, \pi]^2$  and  $(\mathbf{c}_0, \mathbf{b}_0) \in \mathfrak{H}_\varepsilon \setminus \{0\}$ ,

$$\|(\mathbf{1}_{L^2([-\pi, \pi]^2, \mathbf{m}; \mathbb{C})} - P^{(1)}) \hat{\mathbf{c}}_0(k)\|_2 \leq \varepsilon D \|\hat{\mathbf{c}}_0(k)\|_2 .$$

By (62) and (84) together with Proposition 13 (i), the assertion then follows.  $\square$

The existence of the negative eigenvalue  $E(k)$  of  $A(k)$  is not clear in general. Therefore, we define the function  $E^{\text{ext}}(k)$  for all  $k \in [-\pi, \pi]^2$  by  $E^{\text{ext}}(k) := E(k)$  if there is a negative eigenvalue of  $A(k)$  and  $E^{\text{ext}}(k) := 0$  otherwise. To simplify notation, we set  $E^{\text{ext}}(k) \equiv E(k)$ . [By Kato's perturbation theory for the discrete spectrum of closed operators together with Equation (49) and the continuity of  $\hat{v}$ , the map  $k \mapsto E(k)$  from  $[-\pi, \pi]^2$  to  $\mathbb{R}_0^-$  is continuous. This information is not important in the sequel.]

Recall (24), that is,

$$\mathfrak{K}_v := \{k \in [-\pi, \pi]^2 : |\hat{v}(k)| = \|\hat{v}\|_\infty\} .$$

This set can be seen as being the set of quasi-momenta of minimal energy, up to some small errors when  $\varepsilon^{-1}, U \rightarrow \infty$ :

**Lemma 20 (Quasi-momenta of minimal energy at large  $\epsilon^{-1}, U$ )**

Assume that  $|\mathfrak{K}_v| < \infty$ . For any  $\eta > 0$ , there are  $\varepsilon > 0$  and  $D < \infty$  such that, for all  $\epsilon^{-1}, U \geq D$  and all  $k \in [-\pi, \pi)^2 \setminus \{\mathfrak{K}_v + B(0, \eta)\}$ ,

$$E(k) \geq (1 - \varepsilon) \inf E([- \pi, \pi)^2) .$$

*Proof.* Assume without loss of generality that  $\|\hat{v}\|_\infty > 0$ . For any  $\eta > 0$ , there is  $\varepsilon > 0$  such that, for all  $k \in [-\pi, \pi)^2 \setminus \{\mathfrak{K}_v + B(0, \eta)\}$ ,

$$|\hat{v}(k)| \leq (1 - \varepsilon) \max_{k \in [-\pi, \pi)^2} |\hat{v}(k)| , \quad (85)$$

by continuity of  $\hat{v}$ . Indeed, assume the existence of  $\eta > 0$  such that, for all  $\varepsilon > 0$ , there would exist  $k_\varepsilon \in [-\pi, \pi)^2 \setminus \{\mathfrak{K}_v + B(0, \eta)\}$  so that

$$|\hat{v}(k_\varepsilon)| > (1 - \varepsilon) \max_{k \in [-\pi, \pi)^2} |\hat{v}(k)| .$$

By compacticity of  $[-\pi, \pi]^2$  and continuity of  $\hat{v}$ , there is  $k_0 \in [-\pi, \pi)^2 \setminus \{\mathfrak{K}_v + B(0, \eta)\}$  with

$$|\hat{v}(k_0)| = \max_{k \in [-\pi, \pi)^2} |\hat{v}(k)| .$$

Therefore, for any  $\eta > 0$ , there is  $\varepsilon > 0$  such that, for all  $k \in [-\pi, \pi)^2 \setminus \{\mathfrak{K}_v + B(0, \eta)\}$ , (85) holds true, which, combined with Corollary 18 (i), yields the assertion.  $\square$

For any  $k \in [-\pi, \pi)^2$ , let  $\tilde{P}_{\mathfrak{d}(k)}$  be the orthogonal projection acting on the Hilbert space  $L^2([- \pi, \pi)^2, \mathfrak{m}; \mathbb{C}) \times \mathbb{C}$  with

$$\text{Ran}(\tilde{P}_{\mathfrak{d}(k)}) = \mathbb{C} \left( \frac{e^\kappa}{2} \mathfrak{d}(k), \text{sgn}(\hat{v}(k)) \right) .$$

Recall that  $e^\kappa = 2\|\mathfrak{d}(k)\|_2^{-1}$ . Then, for all  $\varepsilon > 0$ , define the projections

$$\mathcal{P}_\varepsilon := \int_{[-\pi, \pi)^2}^{\oplus} \mathbf{1}_{[E_0, E_0(1-\varepsilon)]}(E(k)) \tilde{P}_{\mathfrak{d}(k)} \mathfrak{m}(d^2k)$$

and, for any  $k \in [-\pi, \pi)^2$  and  $\eta, \varepsilon > 0$ ,

$$\tilde{\mathcal{P}}_{\varepsilon, \eta}(k) := \int_{[-\pi, \pi)^2}^{\oplus} \chi_{\varepsilon, \eta}^{(k)}(q) \tilde{P}_{\mathfrak{d}(k)} \mathfrak{m}(d^2q) . \quad (86)$$

where, for any  $q \in [-\pi, \pi]^2$ ,

$$\chi_{\varepsilon, \eta}^{(k)}(q) := \mathbf{1}_{[E_0, E_0(1-\varepsilon)]}(E(q)) \mathbf{1}_{k+B(0, \eta)}(q). \quad (87)$$

These operators are used to approximate now the spectral projection

$$\mathbf{1}_{[E_0, E_0(1-\varepsilon)]}(H^{(2,1)})$$

of the Hamiltonian  $H^{(2,1)}$  on the bottom  $[E_0, E_0(1-\varepsilon)]$  of its spectrum for any parameter  $\varepsilon \in (0, 1)$ .

**Proposition 21 (Approximating projectors)**

Let  $\varepsilon \in (0, 1)$  and assume that  $E_0 < 0$ . For any  $\eta > 0$ , there is a constant  $D < \infty$  such that, for all  $\varepsilon^{-1}, U \geq D$ ,

$$\left\| \mathbf{1}_{[E_0, E_0(1-\varepsilon)]}(H^{(2,1)}) - \mathcal{P}_\varepsilon \right\|_{\text{op}} \leq \eta.$$

Moreover, if  $|\mathfrak{K}_v| < \infty$  and  $\varepsilon \ll 1$  is sufficiently small, then

$$\left\| \mathbf{1}_{[E_0, E_0(1-\varepsilon)]}(H^{(2,1)}) - \sum_{k \in \mathfrak{K}_v} \tilde{\mathcal{P}}_{\varepsilon, \eta}(k) \right\|_{\text{op}} \leq \eta.$$

*Proof.* By Lemma 7 and Proposition 25 (iii),

$$\mathbf{1}_{[E_0, E_0(1-\varepsilon)]}(H^{(2,1)}) = \int_{[-\pi, \pi]^2}^{\oplus} \mathbf{1}_{[E_0, E_0(1-\varepsilon)]}(A(k)) \mathfrak{m}(d^2 k). \quad (88)$$

and the assertion follows by using Theorem 12, Corollary 18 (ii) and Lemma 20. Note that  $E_0 < 0$  yields  $\|\hat{v}\|_\infty > 0$ , by Lemma 9.  $\square$

Recall that the function  $\mathbf{s}_k : \mathbb{Z}^2 \rightarrow \mathbb{C}$  is defined, for any  $k \in [-\pi, \pi]^2$ , by (23), that is,

$$\mathbf{s}_k(y) := \frac{1}{2} \left( e^{ik \cdot (0,1)} \delta_{y, (0,1)} + e^{ik \cdot (0,-1)} \delta_{y, (0,-1)} + e^{ik \cdot (1,0)} \delta_{y, (1,0)} + e^{ik \cdot (-1,0)} \delta_{y, (-1,0)} \right)$$

for all  $y \in \mathbb{Z}^2$ . For any  $\eta, \varepsilon > 0$ ,  $k \in [-\pi, \pi]^2$  and  $y \in \mathbb{Z}^2$ , let

$$\begin{aligned} g_{\varepsilon, \eta}^{(k)}(y) &:= \frac{1}{2} \int_{[-\pi, \pi]^2} \mathfrak{m}(d^2 q) \chi_{\varepsilon, \eta}^{(k)}(q) e^{iq \cdot y} \int_{[-\pi, \pi]^2} \mathfrak{m}(d^2 p) \cos(p - k) [\hat{\mathbf{c}}(q)](p) \\ &\quad + \frac{\text{sgn}(\hat{v}(k))}{2} \int_{[-\pi, \pi]^2} \mathfrak{m}(d^2 q) \chi_{\varepsilon, \eta}^{(k)}(q) e^{iq \cdot y} \hat{\mathbf{b}}(q) \end{aligned}$$

with  $\chi_{\varepsilon, \eta}^{(k)}$  defined by (87). These functions are important because they are directly related to the projections (86):



**Lemma 22 (Range of projections  $\tilde{\mathcal{P}}_{\varepsilon,\eta}$ )**

For any  $(\mathbf{c}, \mathbf{b}) \in \mathcal{H}_{\uparrow,\downarrow}^{(2,1)}$ ,  $\eta, \varepsilon > 0$ ,  $k \in [-\pi, \pi)^2$ ,

$$\left[ \mathfrak{U}^* \tilde{\mathcal{P}}_{\varepsilon,\eta}(k) \mathfrak{U} \right] (\mathbf{c}, \mathbf{b}) = (\mathbf{c}', \mathbf{b}') ,$$

where, for any  $x_\uparrow, x_\downarrow \in \mathbb{Z}^2$ ,

$$\mathbf{c}'(x_\uparrow, x_\downarrow) = \mathbf{s}_k(x_\uparrow - x_\downarrow) g_{\varepsilon,\eta}^{(k)}(x_\uparrow)$$

and, for any  $x_b \in \mathbb{Z}^2$ ,

$$\begin{aligned} \mathbf{b}'(x_b) &= \frac{1}{2} \int_{[-\pi,\pi)^2} \mathbf{m}(\mathrm{d}^2 q) e^{iq \cdot x_b} \chi_{\varepsilon,\eta}^{(k)}(q) \hat{\mathbf{b}}(q) + \frac{\text{sgn}(\hat{v}(k))}{2} \int_{[-\pi,\pi)^2} \mathbf{m}(\mathrm{d}^2 q) \\ &\quad \times e^{iq \cdot x_b} \chi_{\varepsilon,\eta}^{(k)}(q) \int_{[-\pi,\pi)^2} \mathbf{m}(\mathrm{d}^2 k_{\uparrow\downarrow}) \cos(k_{\uparrow\downarrow} - k) [\hat{\mathbf{c}}(q)](k_{\uparrow\downarrow}) . \end{aligned}$$

*Proof.* Fix all the parameters of the lemma. We then compute from (86)–(87) that

$$\begin{aligned} \mathbf{c}'(x_\uparrow, x_\downarrow) &= \frac{1}{2} \left( \int_{[-\pi,\pi)^2} e^{ik_{\uparrow\downarrow} \cdot (x_\downarrow - x_\uparrow)} \cos(k_{\uparrow\downarrow} - k) \mathbf{m}(\mathrm{d}^2 k_{\uparrow\downarrow}) \right) \\ &\quad \times \int_{[-\pi,\pi)^2} \mathbf{m}(\mathrm{d}^2 q) \chi_{\varepsilon,\eta}^{(k)}(q) e^{iq \cdot x_\uparrow} \\ &\quad \left( \text{sgn}(\hat{v}(k)) \hat{\mathbf{b}}(q) + \int_{[-\pi,\pi)^2} \mathbf{m}(\mathrm{d}^2 p) \cos(p - k) [\hat{\mathbf{c}}(q)](p) \right) , \end{aligned}$$

while, for all  $y \in \mathbb{Z}^2$ ,

$$\int_{[-\pi,\pi)^2} e^{ik_{\uparrow\downarrow} \cdot y} \cos(k_{\uparrow\downarrow} - k) \mathbf{m}(\mathrm{d}^2 k_{\uparrow\downarrow}) = \mathbf{s}_k(y) , \quad (89)$$

by using (19). A similar computation can be done for  $\mathbf{b}'$ . We omit the details.  $\square$

For any  $k \in [-\pi, \pi)^2$ , let the orthogonal projection  $P_{\mathfrak{h}_{2,-}^{(0)}}$  acting on  $\mathcal{H}_{\uparrow,\downarrow}^{(2,1)}$  with range  $\mathfrak{h}_{2,-}^{(0)}$ . Recall that  $\mathfrak{h}_{2,-}^{(0)}$  is the subspace of one zero-spin electron pair, which is canonically isomorphic to the spaces (12). Then, we can see a 50% depletion of either the fermion pair density or the boson density for large  $\epsilon^{-1}, U$  (cf. (22)):

**Lemma 23 (Bosonic depletion at large  $\epsilon^{-1}, U$ )**

Let  $\varepsilon \in (0, 1)$  and assume that  $E_0 < 0$ . Then, uniformly for all normalized vectors  $\psi \in \mathcal{H}_{\uparrow, \downarrow}^{(2,1)}$ ,

$$\lim_{\epsilon^{-1}, U \rightarrow \infty} \left| \left\| P_{\mathfrak{h}_{2,-}^{(0)}} \mathbf{1}_{[E_0, E_0(1-\varepsilon)]} (H^{(2,1)}) \psi \right\|_{\mathcal{H}_{\uparrow, \downarrow}^{(2,1)}} - \frac{1}{\sqrt{2}} \left\| \mathbf{1}_{[E_0, E_0(1-\varepsilon)]} (H^{(2,1)}) \psi \right\|_{\mathcal{H}_{\uparrow, \downarrow}^{(2,1)}} \right| = 0 .$$

*Proof.* It is direct consequence of Corollary 18 (ii) and Equation (88).  $\square$

## 5.5 Effective Fermi Model

Similar to the three-body case studied above, the fermionic effective Hamiltonian

$$\tilde{H}^{(2,1)} := \overline{\tilde{\mathbf{H}}|_{\mathcal{H}_{\uparrow, \downarrow}^{(2,1)}}} ,$$

which is defined by (30), is decomposable:

$$\mathfrak{U}^* \tilde{H}^{(2,1)} \mathfrak{U} = \int_{[-\pi, \pi]^2}^{\oplus} \tilde{A}_{1,1}(k) \oplus \tilde{A}_{2,2}(k) \, \mathfrak{m}(\mathrm{d}^2 k) , \quad (90)$$

where, for any  $k \in [-\pi, \pi]^2$ ,

$$\tilde{A}_{1,1}(k) := A_{1,1}(k) - (1 + 4e^{-2\kappa}) \hat{w}_f(k) P_{\mathfrak{d}(k)} , \quad \tilde{A}_{2,2}(k) := -\hat{w}_b(k) , \quad (91)$$

with  $\hat{w}_b$  and  $\hat{w}_f$  being the Fourier transforms of  $w_b$  (27) and  $w_f$  (29), respectively. See also (42) for the definition of  $A_{1,1}(k)$  and recall that  $P_{\mathfrak{d}(k)}$  is the orthogonal projection with range (39). The fiber decomposition of  $\mathfrak{U}^* \tilde{H}^{(2,1)} \mathfrak{U}$  is obtained by direct computations and we omit the details.

The bosonic and fermionic subspaces are clearly invariant under the action of  $\tilde{H}^{(2,1)}$ . Eigenvalues and eigenvectors of  $\tilde{A}_{2,2}(k)$ ,  $k \in [-\pi, \pi]^2$ , do not need to be discussed as these operators act on one-dimensional spaces. Thus, we focus on the fermionic subspace. Here, by (29),  $\hat{w}_f(k) \geq 0$  and we can use the Birman–Schwinger principle (Proposition 26) once again with

$$H_0 = A_{1,1}(k) \quad \text{and} \quad V = (1 + 4e^{-2\kappa}) \hat{w}_f(k) P_{\mathfrak{d}(k)} ,$$

to study the negative eigenvalues of  $\tilde{A}_{1,1}(k)$ : Let  $k \in [-\pi, \pi]^2$ . Then,  $\lambda < 0$  is an eigenvalue of  $\tilde{A}_{1,1}(k)$  if and only if

$$\hat{w}_f(k) \mathcal{R}(k, U, \lambda) = 1 \quad (92)$$

with  $\mathcal{R}(k, U, \lambda)$  defined by (54). Moreover, this eigenvalue is non-degenerated and unique, by Lemma 11. Note that, by compacticity of  $P_{\mathfrak{d}(k)}$  and  $\tilde{A}_{2,2}(k)$  as well as the positivity of  $A_{1,1}(k)$ , any strictly negative eigenvalue of  $\tilde{A}_{2,2}(k)$  is discrete. Comparing the last equation with Proposition 10 and Corollary 18,  $w_f$  (29) is chosen such that the negative eigenvalues  $\tilde{E}(k)$  and  $E(k)$  of  $\tilde{A}_{1,1}(k)$  and  $A(k)$ , respectively, coincide in the limit  $\epsilon \rightarrow 0^+$  and  $U \rightarrow \infty$ . Indeed, we tune the parameter  $\gamma_f > 0$  in (29) in order to maximize the rate of convergence of

$$|\tilde{E}(k) - E(k)| \rightarrow 0 ,$$

as  $\epsilon \rightarrow 0^+$ ,  $U \rightarrow \infty$ , and we obtain the following result:

**Proposition 24 (Asymptotics of the negative eigenvalue of  $\tilde{A}_{1,1}(k)$ )**

Let  $\gamma_f = e^\kappa/2$ . Then, there is a constant  $D_\kappa < \infty$  depending only on  $\kappa > 0$  such that, for all  $k \in [-\pi, \pi)^2$ ,  $\epsilon \geq 0$  satisfying  $2\epsilon \leq \tilde{\epsilon}_0 |\hat{v}(k)|$ , and every  $U \geq 0$ , one has:

(i) There is a unique negative eigenvalue  $\tilde{E}(k)$  of  $\tilde{A}_{1,1}(k)$ . Moreover, it is non-degenerated and satisfies

$$\left| \tilde{E}(k) + 2e^{-\kappa} |\hat{v}(k)| + \frac{|\hat{v}(k)|^2}{2U} \right| \leq D_\kappa (\epsilon + U^{-2}) .$$

(ii) There is an eigenvector  $\tilde{\Psi}_{\uparrow\downarrow}(k)$  associated with  $\tilde{E}(k)$  satisfying

$$\left\| \tilde{\Psi}_{\uparrow\downarrow}(k) - \frac{e^\kappa}{2} \text{sgn}(\hat{v}(k)) \mathfrak{d}(k) - \frac{\hat{v}(k)}{U} \mathfrak{s} \right\|_2 \leq D_\kappa (\epsilon |\hat{v}(k)|^{-1} + U^{-2}) .$$

*Proof.* By (29) for  $\gamma_f = e^\kappa/2$  and (42), note that

$$\tilde{A}_{1,1}(k) = A_{1,1}(k) - \frac{e^\kappa}{2} (1 + 4e^{-2\kappa}) \left( |\hat{v}(k)| - \frac{e^\kappa}{4U + 2} |\hat{v}(k)|^2 \right) P_{\mathfrak{d}(k)} .$$

Therefore, similar to Theorem 16, it suffices to study the operator

$$UP_0 - \frac{e^\kappa}{2} (1 + 4e^{-2\kappa}) \left( |\hat{v}(k)| - \frac{e^\kappa}{4U + 2} |\hat{v}(k)|^2 \right) P_{\mathfrak{d}(k)}$$

for large  $U \geq 0$ . Explicit computations shows in this case that the negative eigenvalue of the last operator is

$$\begin{aligned} \tilde{F}(k) := & \left( \frac{|\hat{v}(k)|}{2} - \frac{e^\kappa}{8U+4} |\hat{v}(k)|^2 \right) \left( \frac{U}{|\hat{v}(k)| - \frac{e^\kappa}{4U+2} |\hat{v}(k)|^2} - \left( \frac{e^\kappa}{2} + 2e^{-\kappa} \right) \right. \\ & \left. - \sqrt{\left( \frac{U}{|\hat{v}(k)| - \frac{e^\kappa}{4U+2} |\hat{v}(k)|^2} + 2e^{-\kappa} - \frac{e^\kappa}{2} \right)^2 + 4} \right) \end{aligned} \quad (93)$$

with associated eigenvector  $\tilde{\Phi}_{\uparrow\downarrow}(k)$  equal to

$$\tilde{\Phi}_{\uparrow\downarrow}(k) = \left( \frac{|\hat{v}(k)|}{-\tilde{F}(k)} + \frac{|\hat{v}(k)|}{U} \right) \mathfrak{d}(k) + \frac{|\hat{v}(k)|}{U} \mathfrak{s} . \quad (94)$$

Then, direct estimates from (93)–(94) imply Assertions (i)–(ii). Note that, in order to use Kato's perturbation theory as in Theorem 16 we need the estimate  $\tilde{E}(k) = \mathcal{O}(1)$ , uniformly with respect to  $U \geq 0$ , which is deduced from (92) as in Theorem 12 for  $E(k)$ .  $\square$

## 6 Appendix

### 6.1 Direct Integral Decomposition

For more details, we refer to [23, Section XIII.16].

Let  $(\mathfrak{M}, \mathfrak{m})$  be any  $\sigma$ -finite measure space and  $(\mathcal{H}, \langle \cdot, \cdot \rangle_{\mathcal{H}})$  any separable Hilbert space. The constant fiber direct integral

$$\int_{\mathfrak{M}}^{\oplus} \mathcal{H} \, \mathfrak{m}(\mathrm{d}x)$$

is denoted by  $L^2(\mathfrak{M}, \mathfrak{m}; \mathcal{H})$  and corresponds to the usual Hilbert space of  $\mathcal{H}$ -valued functions on  $\mathfrak{M}$  with scalar product

$$\langle f, g \rangle := \int_{\mathfrak{M}} \langle f(x), g(x) \rangle_{\mathcal{H}} \, \mathfrak{m}(\mathrm{d}x) .$$

Recall that we denote the Banach space of bounded operators acting on  $\mathcal{H}$  by  $\mathcal{B}(\mathcal{H})$  with operator norm  $\| \cdot \|_{\text{op}}$ . A map  $A(\cdot)$  from  $\mathfrak{M}$  to  $\mathcal{B}(\mathcal{H})$  is called

*measurable* if and only if the map  $x \mapsto \langle \psi_1, A(x)\psi_2 \rangle$  from  $\mathfrak{M}$  to  $\mathbb{R}$  is measurable for all  $\psi_1, \psi_2 \in \mathcal{H}$ .

Let  $L^\infty(\mathfrak{M}, \mathfrak{m}; \mathcal{B}(\mathcal{H}))$  be the space of equivalence classes of measurable functions  $A : \mathfrak{M} \rightarrow \mathcal{B}(\mathcal{H})$  with

$$\|A\|_\infty := \text{ess sup } \|A(\cdot)\|_{\text{op}} < \infty .$$

A bounded operator  $A$  on  $L^2(\mathfrak{M}, \mathfrak{m}; \mathcal{H})$  is *decomposable* or *decomposed* by the direct integral decomposition if and only if there is  $A(\cdot) \in L^\infty(\mathfrak{M}, \mathfrak{m}; \mathcal{B}(\mathcal{H}))$  such that

$$(A\Psi)(x) = A(x)\Psi(x) , \quad \Psi \in L^2(\mathfrak{M}, \mathfrak{m}; \mathcal{H}) .$$

The operators  $A(x) \in \mathcal{B}(\mathcal{H})$  are the so-called fibers of  $A$  and we write

$$A = \int_{\mathfrak{M}}^{\oplus} A(x) \, \mathfrak{m}(dx) .$$

The space of decomposable operators can be isometrically identified with the space  $L^\infty(\mathfrak{M}, \mathfrak{m}; \mathcal{B}(\mathcal{H}))$ . See, e.g., [23, Theorem XIII.83]. [23, Theorem XIII.85] also gives properties of self-adjoint operators on the space  $L^\infty(\mathfrak{M}, \mathfrak{m}; \mathcal{B}(\mathcal{H}))$  in terms of its fibers. Only [23, Theorem XIII.85 (a), (c), (d)] is used in this paper and so, for the reader's convenience, we reproduce it below:

**Proposition 25 (Self-adjoint decomposition)**

Let  $A \in L^\infty(\mathfrak{M}, \mathfrak{m}; \mathcal{B}(\mathcal{H}))$  with  $A(x)$  being self-adjoint for any  $x \in \mathfrak{M}$ . Then:

- (i)  $A$  is self-adjoint with spectrum  $\sigma(A)$ .
- (ii)  $\lambda \in \sigma(A)$  if and only if, for all  $\varepsilon > 0$ ,

$$\mathfrak{m}(\{x \in \mathfrak{M} : \sigma(A(x)) \cap (\lambda - \varepsilon, \lambda + \varepsilon) \neq \emptyset\}) > 0 .$$

- (iii) For any bounded Borel function  $f$  on  $\mathbb{R}$ ,

$$f(A) = \int_{\mathfrak{M}}^{\oplus} f(A(x)) \, \mathfrak{m}(dx) .$$

## 6.2 The Birman–Schwinger Principle

There are various versions of the Birman–Schwinger principle. The following one is used in our proofs:

**Proposition 26 (Birman–Schwinger principle)**

Let  $d \geq 1$  and  $H_0, V \in \mathcal{B}(\ell^2(\mathbb{Z}^d))$  be positive bounded operators. Assume further that  $V$  is compact. For any  $\lambda < 0$ , define the compact, self-adjoint, positive Birman–Schwinger operator by

$$B(\lambda) = B(\lambda, H_0, V) := V^{1/2} (H_0 - \lambda)^{-1} V^{1/2} .$$

Then  $\lambda < 0$  is an eigenvalue of  $(H_0 - V)$  of multiplicity  $M$  if and only if 1 is an eigenvalue of  $B(\lambda)$  of multiplicity  $M$ .

*Proof:* We recall that, due to the compactness of  $V$ , the Birman–Schwinger operator  $B(\lambda)$  is compact and has only discrete spectrum above 0. Similarly, the spectrum of  $(H_0 - V)$  below 0 is discrete because  $V$  is compact.

Suppose that  $\lambda < 0$  is an eigenvalue of  $(H_0 - V)$  of multiplicity  $M \in \mathbb{N}$  and let  $\{\varphi_1, \dots, \varphi_M\} \subseteq \ell^2(\mathbb{Z}^d)$  be an orthonormal basis (ONB) of the corresponding eigenspace. Set

$$\psi_1 := V^{1/2} \varphi_1, \dots, \psi_M := V^{1/2} \varphi_M \in \ell^2(\mathbb{Z}^d) . \quad (95)$$

Then

$$\varphi_m = (H_0 - \lambda)^{-1} V \varphi_m = (H_0 - \lambda)^{-1} V^{1/2} \psi_m , \quad (96)$$

and the boundedness of  $(H_0 - \lambda)^{-1} V^{1/2}$  implies that  $\{\psi_1, \dots, \psi_M\} \subseteq \ell^2(\mathbb{Z}^d)$  is a linearly independent family. Clearly, (95) and (96) also yield

$$B(\lambda) \psi_m = V^{1/2} (H_0 - \lambda)^{-1} V^{1/2} \psi_m = \psi_m , \quad (97)$$

and hence the eigenspace of  $B(\lambda)$  corresponding to the eigenvalue 1 has at least dimension  $M$ .

Conversely, if  $\{\psi_1, \dots, \psi_L\} \subseteq \ell^2(\mathbb{Z}^d)$  is an ONB of the eigenspace of  $B(\lambda)$  corresponding to the eigenvalue 1 of multiplicity  $L \in \mathbb{N}$  then we set

$$\varphi_1 := (H_0 - \lambda)^{-1} V^{1/2} \psi_1, \dots, \varphi_L := (H_0 - \lambda)^{-1} V^{1/2} \psi_L \in \ell^2(\mathbb{Z}^d) . \quad (98)$$

Then,

$$\psi_k = B(\lambda) \psi_k = V^{1/2} \varphi_k , \quad (99)$$

and the boundedness of  $V^{1/2}$  implies that  $\{\varphi_1, \dots, \varphi_L\} \subseteq \ell^2(\mathbb{Z}^d)$  is a linearly independent family. Clearly, (98) and (99) also yield

$$(H_0 - V) \varphi_k = \lambda \varphi_k , \quad (100)$$

and hence the eigenspace of  $(H_0 - V)$  corresponding to the eigenvalue  $\lambda$  has at least dimension  $L$ .  $\square$

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